13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Phase-Field Modeling of the \Alpha-\Gamma Phase Transformation of RDX

Author(s): Rahul ., Suvranu De, *RPI*.

RDX is an extensively used energetic material that undergoes \alpha-\gamma phase transformation in the pressure range of 3.5-4.5 GPa [1]. The \alpha-\gamma phase transition involves a decrease in unit cell volume of about 3% and leads to changes in the space group and molecular conformations [2] that likely serve to precondition the material for the onset of initiation at higher stresses. Understanding and predicting the effect of phase transformations on initiation and the critical parameters for transition to detonation under intended or unintended thermomechanical stimuli have therefore been an important and challenging problem. At its heart is the need to understand the complex deformation processes by which localization of energy can lead to regions in the material with sufficiently high temperature and stress conditions to promote rapid molecular decomposition. We develop a thermodynamically consistent continuum phase field model to investigate the role of shock-induced \alpha-\gamma phase transition in the sensitivity of RDX. Dislocations and phase transformations are distinguished and modeled within a crystal plasticity framework. The Landau potential is derived for the finite elastic deformation analysis. The shock-response of RDX crystal is obtained by solving the continuum momentum equation along with phase evolution equation using a Helmholtz free energy functional, which consists of elastic potential energy and local interfacial energy that follows from the Cahn–Hilliard formalism [3]. We observe that the orientations for which there is a resolved shear stress along the slip direction, the material absorbs large shear strain through plastic deformation, allowing it to be less sensitive as less mechanical work is available for temperature rise. Therefore, plastic slip should be associated with greater shear relaxation and, hence, decreased sensitivity. For elastic orientations, large shear stress arises from steric hindrance that may provides much more mechanical work to increase the temperature and hence more sensitive to detonation. Our simulations suggest that the \alpha-\gamma phase transformation in RDX may be associated with the increased temperature rise and hence the shock sensitivity. References 1. Z. A. Dreger, Y. M. Gupta, J. Phys. Chem. A 114, 8099 (2010). 2. Z. A. Dreger, J. E. Patterson, Y. M. Gupta, J. Phys. Conf. Ser. 121, 042012 (2008). 3. J. Cahn, J. Hilliard, J. Chem. Phys. 28, 258 (1958).

13th U.S. National Congress on Computational Mechanics
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Title: Phase-Field Simulations of Eutectic Alloy Solidification into Templates for Photonic Metamaterials

Author(s): Larry Aagesen, Ali Ramazani, Katsuyo Thornton, *U. Michigan*; Jinwoo Kim, Paul Braun, *U. Illinois Urbana-Champaign*.

Photonic metamaterials are multi-phase materials that have a structure with periodicity smaller than the wavelength of light. These metamaterials can be used to create optical responses not possible in nature, such as negative refractive indices. A novel approach to create photonic metamaterials is the solidification of eutectic alloys into inert templates with periodic geometries to control the long-range periodicity of the solidified eutectic microstructure. In this approach, both the periodic structure of the eutectic alloy itself (lamellae or rods) and the periodicity of the template affect light-matter interactions. We have developed a phase-field model to simulate the effects of various template geometries on the structure of solidifying eutectic alloys. The smoothed boundary method (SBM) is used to include template-eutectic interactions in the system. This method allows an arbitrarily complex template geometry to be represented, and enforces a no-flux boundary condition at the interface between the template and the solidifying eutectic. The model is applied to a lamellar AgCl-KCl eutectic, which solidifies into an “artificial opal” template, an array of silica spheres with face-centered cubic ordering. The effect of varying template sphere diameter and solidification conditions is explored, and simulation results are compared to experiment.

13th U.S. National Congress on Computational Mechanics
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Title: The Fluid-Structure Interaction Technique Specialized to Axially-Symmetric Objects

Author(s): Ahmad Abawi, *HLS Research*; Petr Krysl, *UC San Diego*.

The fluid-structure interaction technique provides a paradigm for solving scattering from elastic objects embedded in a fluid by a combination of finite and boundary element methods. In this technique, the finite element method is used to compute the object's impedance matrix and the Helmholtz-Kirchhoff integral with the appropriate Green's function is used to represent the field in the exterior medium. The two equations are coupled at the surface of the object by imposing the continuity of pressure and normal displacement. This results in a Helmholtz-Kirchhoff boundary element equation that can be used to compute the scattered field anywhere in the surrounding environment. This method reduces a finite element problem to a boundary element one with drastic reduction in the number of unknowns, which translates to a significant reduction in numerical cost. This method was developed and tested for general 3D objects. In this paper the method is specialized to axially symmetric objects, which provides further reduction in numerical cost, and validated using benchmark solutions.

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Title: Uniaxial Compression of Random Discontinuous Long-Fiber Thermoplastics: Direct Simulation

Author(s): Ahmed Abd El-Rahman, *Cairo U.*; Charles Tucker III, *U. Illinois, Urbana-Champaign*.

The mechanical interactions between fibers in a dense random-fiber network transmit stress, cause fiber curvature, and influence fiber orientation in the processing of many types of composites. A few theories describe the mechanics of fiber networks, but almost no simulation results are available. Here, we report a direct numerical simulation of the mechanical behavior of random-fiber networks. The finite element method is used, and each fiber is represented by a small number of 3-D beam elements. The calculations assume a periodic structure to avoid boundary effects, but within the unit cell, the fibers are placed randomly. A special algorithm that uses the random sequential adsorption process creates an initial structure of straight, random, non-intersecting fibers from which a unit cell with periodic boundary conditions is built automatically [A. I. Abd El-Rahman and C. L. Tucker III, ASME J. Appl. Mech., 2013]. The simulation uses an explicit time integration of dynamic equations, with a general contact algorithm (ABAQUS/Explicit). A typical run involves 5000 fibers with l/d = 100, compressing the network from an initial volume fraction of 5% to a final volume fraction of 25% using 10^5 time steps. At the final volume fraction, there are 200 000 fiber-fiber contacts. Results from the simulation are in good agreement with van Wyk [J. Text. Inst. 37, 1946] theory for compaction pressure at low-to-moderate fiber density. They show fair agreement with Toll [Polym. Eng. Sci. 38(8), 1998] theory for the number of fiber-fiber contacts, and they also show good agreement with a simple slender-body model for fiber orientation, at least during the initial uniaxial compression. This simulation provides an interesting tool for understanding the mechanics of random-fiber networks and building models of composite materials processing.

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Title: Grain Boundary Faceting in the Presence of Junction Dislocations: A Phase Field Treatment

Author(s): Fadi Abdeljawad, Douglas Medlin, Jonathan Zimmerman, Khalid Hattar, Stephen Foiles, *Sandia Nat'l. Labs.*.

A detailed understanding of interfaces and their interactions with other defects holds the key to the future development of increasingly complex materials systems. As the characteristic length scale of a materials system gets smaller, the role of interfaces becomes even more profound owing to their high densities in such systems. Thermodynamically, the equilibrium shape of a crystal minimizes the total interfacial energy and the classic Wulff construction provides a treatment for the dependence of the equilibrium shape on interface anisotropy. For strongly anisotropic interfaces, it may be thermodynamically favorable for an interface to evolve and exclude a range of orientations leading to the formation of corners and facets. In a polycrystalline metal and for a given orientation of two adjoining crystals, cusps in the grain boundary (GB) energy may exist as a function of GB inclination, indicating the presence of low energy planes. Therefore, an initially flat GB may facet resulting in a “hill and valley” structure corresponding to these low energy planes. Additionally, we consider the general case, where dislocations exist at GB facet junctions due to differences in the translation states at these intersecting facets. The contribution to the total energy by junction dislocations along with their nonlocal elastic interactions may affect facet coarsening and the resulting characteristic facet length scale. In this talk, we present a phase field model for GB faceting in the presence of junction dislocations. The modeling framework accounts for anisotropic GB energy, junction dislocations and their nonlocal elastic interactions, and incorporates corner energy regularization for facet coarsening. Simulation results of several model systems are presented to demonstrate the capability of the model and infer regimes, where stabilization of GB facets occurs due to junction dislocations. More specifically, we consider the case of a &Sigma =5 <001> tilt boundary in BCC iron, where we have experimentally investigated facets along {210} and {310} planes using high resolution scanning transmission electron microscopy. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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Title: Efficiency of High-Order Methods in Space and Time: Study of Elastodynamics Problem Using Spacetime Discontinuous Galerkin Finite Element Method

Author(s): Reza Abedi, Omid Omidi, *U. Tennessee Space Inst.*; Scott Miller, *Penn. State U.*; Robert Haber, *U. Illinois, Urbana-Champaign*.

Generally, higher order methods refer to third order or higher [1]. Two general beliefs that have resulted in more widespread use of lower order methods in academia and especially in industry are [1]: 1) Higher order methods are more expensive; 2) They are not needed for engineering accuracies. Referring to the former, efficiency is a better measure than solution cost. To investigate a method's efficiency both error convergence rate and solution cost scaling versus number of elements and element order should be well-understood. While the former generally has a simple power form, the solution cost scaling is much more complicated and highly dependent on particular formulation of a finite element method (FEM). For example as a result of the global coupling of conventional continuous FEMs, [2] reports that even for 0.1% relative accuracies—which is tenfold the commonly used 1% range in many engineering applications—linear elements are more efficient than higher order elements for realistic 3D applications. We investigate when higher order methods are more efficient in the context of a highly advanced spacetime discontinuous Galerkin (SDG) finite element method [3] where a novel use of characteristic structure of the wave equation in discretization, yields a method with linear solution complexity. Some aspects of our study are: 1) Unlike continuous FEMs the very local solution nature of the SDG method may favor higher order elements. This clearly advocates the use of higher order elements for realistic 3D applications; 2) In many dynamic applications, e.g. wave propagation, temporal order is as important as spatial order. We comment on general challenges in achieving arbitrary high temporal orders—particularly when more efficient non-spatially uniform orders are demanded—and discuss how the SDG method gracefully addresses these issues; 3) We demonstrate multi-field formulations can in fact be more efficient than single-field formulations; 4) An FEM's efficiency is greatly affected by the cost scaling of assembly and the solution of global matrices. We demonstrate this concept through comparison between single-cell and a new multi-cell element formulation. References: [1] Wang, Z.J. et. al., High-order CFD methods: Current status and perspective, Int. J Numer. Meth. Fl., 72(8), 811-845, 2013. [2] Lohner, R., Improved error and work estimates for high-order elements, Int. J Numer. Meth. Fl., 72(11), 1207-1218, 2013. [3] Abedi, R., Haber, R.B., Petracovici b., A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum. Comput. Method Appl. M., 195:3247–3273, 2006.

13th U.S. National Congress on Computational Mechanics
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Title: Microstructure Size Effect Incorporated Crystal Plasticity Constitutive Model for Multi-Phase Polycrystalline Materials

Author(s): Masoud Ghorbani Moghaddam, Ajit Achuthan, *Clarkson U.*.

Multi-phase materials such as Nickel-Based super alloys (ME3) are widely used in various industrial applications due to their exceptional strength, fracture toughness and resistance against creep and corrosion at elevated temperature and other harsh environment. The deformation of the multi-phase materials is influenced by two micro-structural feature sizes; the grain size effect and the precipitate size effect. The classical crystal plasticity constitutive models do not have a mechanism to capture the microstructural length scale effects. In this paper, we discuss the development of a new method to introduce microstructural feature size effects into crystal plasticity constitutive models, and demonstrate the validity of the model by simultaneously capturing both the grain size and the precipitate size dependent behavior of Nickel-based super alloys on a finite element framework. The proposed method relies on introducing a fictitious work-hardenings equivalent to the resistance to dislocation motion in the boundary influence regions (regions near the grain boundary and in the matrix around the precipitate boundary). The fictitious work hardening is introduced as a fictitious pre-existing plastic strain in the boundary influence regions. The introduced work hardening increases the yield stress and the initial hardening coefficient of the grain, and reduces the ability of the material to further work-harden; thus simulating the resistance to dislocation nucleation and motion in the boundary influence regions. The ability of the method to capture the size dependence on both the yield stress (Hall-Petch effect) and the strain hardening modulus, and thus the evolution of stress-strain behavior, are then demonstrated. Two-phase materials in the form of single crystals in different sizes and volume fractions (72.9% and 51.2%) and polycrystalline materials are studied to verify the developed constitutive model. The size of the boundary influence region being constant, the effect of boundary region starts to dominate as the precipitate (for a given volume fraction) or the grain becomes smaller, thereby capturing the Hall-Petch effect.

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Title: Higher-Order Immersed Discontinuous Galerkin Methods for Interface Problems

Author(s): Slimane Adjerid, *Virginia Tech*.

\documentclass[12pt]{article} \usepackage{epsf,exscale,times} \setlength{\parindent}{0pt} \hoffset=-5mm\voffset=-25mm\textwidth=155mm\textheight=250mm %%% \begin{document} \pagestyle{empty} \begin{center} \bf Higher Order Immersed Discontinuous Galerkin Methods for Interface Problems \end{center} \begin{center} \textbf{ Slimane Adjerid*, Kihyo Moon and Tao Lin}\\ \end{center} \begin{center} Department of Mathematics \\ Virginia Tech, Blacksburg \\ VA 24061, USA\\ \emph{adjerids@vt.edu, hyoxt121@vt.edu, tlin@vt.edu} \end{center} \vspace{4mm} We discuss high order immersed finite element (IFE) spaces and methods for two dimensional partial differential equations on nonhomogenous domains without requiring the mesh to be aligned with the material interfaces. We discuss the properties and approximation capabilities of such IFE spaces and show that the interpolation errors in the proposed piecewise p^{th} degree spaces yield optimal $\mathcal{O}(h^{p+1})$ and $\mathcal{O}(h^{p})$ convergence rates in the L^2 and broken H^1 norms, respectively, under mesh refinement. Interior penalty and discontinuous Galerkin methods are used to test the proposed IFE spaces by solving second-order elliptic interface problems, the acoustic interface problem and Stokes problem for multi-phase flow. Several numerical examples are presented to show that the proposed IFE spaces and methods yield optimal convergence rates. \end{document}

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Title: Referential Continuum Fields in Atomistics

Author(s): Nikhil Chandra Admal, *UC Los Angeles*; Ellad Tadmor, *U. Minnesota*.

The various fields defined in continuum mechanics have both a material and a spatial description that are related through the deformation mapping. In contrast, continuum fields defined for atomistic systems using the Irving-Kirkwood or Murdoch-Hardy procedures correspond to a spatial description. Due to the absence of a deformation mapping field in atomistic simulations, it is uncommon to define atomistic fields in the reference configuration. In this paper, we show that the Murdoch-Hardy procedure can be modified to obtain pointwise continuum fields in the reference configuration using the motion of particles as a surrogate for the deformation mapping. These fields identically satisfy the the relations between the referential and the spatial fields given in continuum mechanics. In particular, we obtain definitions for the first and second atomistic Piola-Kirchhoff stress tensors. We demonstrate the validity of these definitions through a numerical example involving finite deformation of a slab containing a notch under tension. An interesting feature of the atomistic first Piola-Kirchhoff stress tensor is the absence of a kinetic part, which in the atomistic Cauchy stress tensor accounts for thermal fluctuations. We show that this effect is implicitly included in the atomistic first Piola-Kirchhoff stress tensor through the motion of the particles.

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Title: Stiffness Update Procedure in Iterative Global-Local Analysis of Columns

Author(s): R. Emre Erkmen, Ashkan Afnani , Vida Niki, *U. Tech-Sydney*.

The purpose of this study is to develop a computationally efficient finite element procedure for the analysis of columns undergoing local deformations. Traditionally, beam-type structural elements are modelled using one dimensional beam finite elements, which are formulated by adopting rigid cross-sectional assumption and therefore cannot capture local/cross-sectional deformations such as local buckling, crack, etc. Such local behaviour can be captured using more sophisticated computationally expensive shell elements. Using the global-local/multi-scale procedure, the size of the model can be optimized by adopting a coarse-scale model for the whole structure while using sufficiently detailed model at the locations where local behaviour is expected [1]. The two models overlap in such regions and are synchronized together using an overlapping decomposition matrix. Consequently, the effect of the local deformations on the global response of the structure can be considered by the additional unbalanced forces exerted on the nodes of the global model. The problem considered herein consists of adopting beam element as the global model and using more sophisticate finite elements capable of capturing localized behaviour in the local regions. The computational problem that arises is that the stiffness matrix is formulated according to the global model, and as a result, considerably large number of iterations is required when the local deformations are significant. To overcome this difficulty, a stiffness update technique is presented in which the displacement field of the global/beam model is altered at each step to consider the locally induced softening behaviour in order to accelerate the convergence. This goal is achieved by introducing embedded discontinuities in the beam element. Within the beam element formulation, these discontinuities are in the form of an internal enrichment considering additional local degrees of freedom associated with the local springs which adjust the stiffness matrix of the beam according to the effects of the local membrane behaviour. These additional degrees of freedom are then eliminated at the element level to achieve a simple assemblage procedure. The efficiency of the proposed model is verified through numerical examples. References 1. Erkmen, RE (2013). Bridging multi-scale approach to consider the effects of local deformations in the analysis of Thin-walled members. Computational Mechanics; 52:65-79.

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Title: Extended Finite-Element Method with Global Enrichment

Author(s): Konstantinos Agathos, *Aristotle U. Thessaloniki; ETH Zurich*; Eleni Chatzi, *ETH Zürich*; Stéphane P. A. Bordas, *U. Luxembourg*; Demosthenes Talaslidis, *Aristotle U. Thessaloniki*.

A variant of the extended finite element method is presented which facilitates the use of enriched elements in a fixed volume around the crack front (geometrical enrichment) in 3D fracture problems. The major problem associated with geometrical enrichment is that it significantly deteriorates the conditioning of the resulting system matrices, thus increasing solution times and in some cases making the systems unsolvable. For 2D problems this can be dealt with by employing degree of freedom gathering [1] which essentially inhibits spatial variation of enrichment function weights. However, for the general 3D problem such an approach is not possible since spatial variation of the enrichment function weights in the direction of the crack front is necessary in order to reproduce the variation of solution variables, such as the stress intensity factors, along the crack front. The proposed method solves the above problem by employing a superimposed mesh of special elements which serve as a means to provide variation of the enrichment function weights along the crack front while still not allowing variation in any other direction. The method is combined with special element partitioning algorithms [2] and numerical integration schemes [3] as well as techniques for the elimination of blending errors between the standard and enriched part of the approximation in order to further improve the accuracy of the produced results. Additionally, a novel benchmark problem is introduced which enables the computation of displacement and energy error norms as well as errors in the stress intensity factors for the general 3D case. Through this benchmark problem it is shown that the proposed method provides optimal convergence rates, improved accuracy and reduced computational cost compared to standard XFEM. REFERENCES 1 Laborde P, Pommier J, Renard Y, Salaün M High-order extended finite element method for cracked domains. International Journal for Numerical Methods in Engineering 2005; 64(3):354-381. 2 Loehnert S, Mueller-Hoeppe DS, Wriggers P 3D corrected XFEM approach and extension to finite deformation theory. International Journal for Numerical Methods in Engineering 2011; 86:431-452. 3 Minnebo H Three■dimensional integration strategies of singular functions introduced by the XFEM in the LEFM. International Journal for Numerical Methods in Engineering 2012; 92:1117–1138.

13th U.S. National Congress on Computational Mechanics
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Title: An Inverse Modeling Framework for Determination of Heart Valves' Mechanical Properties

Author(s): Ankush Aggarwal, Michael Sacks, *UT Austin*.

Heart valves play a very important role in the functioning of the heart and many of the heart failures are related to the valvular dysfunctions, e.g. aortic stenosis and mitral regurgitation. Relationship between the biomechanical properties of valve leaflets and their function has long been established, however, determining these properties in a non-invasive manner remains a challenge. Here we present a framework for such a tool for biomechanical properties determination. We use an inverse-modeling approach, where the only input is through imaging the leaflet tissue as it is loaded naturally during the cardiac cycle. Using a structural model for the leaflet material behavior allows us to reduce the number of parameters to be determined to only two, which in addition to dramatically reducing the computational time also allows one to visualize the cost function and the minimization process. We present results from its application on an in-vitro experimental dataset that was published previously. This allows us to perform a systematic convergence and sensitivity analysis, as well as validate our method against well established biaxial-stress protocol. The cost function is defined in such a way that it is applicable to clinical imaging, which does not provide information about material points. The structural model, like most of the tissue constitutive laws, includes an exponential function to define the ensemble response. We present an analysis of the fitting to exponential functions and show that in such a case many sets of parameters can provide very similar response. We use this aspect to reduce the number of parameters in the optimization process. Simulating a single leaflet rather than a composite valve provides a substantial computational speed-up. Optimizing the inverse-model based on it provides a good first estimate of the mechanical properties, which are further fine-tuned using full simulation-based inverse model. We determine the importance of various structural parameters like the fiber direction and splay in estimating the correct biomechanical properties. The imaging resolution is found to be an important aspect of this setup. We also briefly discuss all of the other constituents needed to make it a clinically viable tool.

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Title: Multi-Time-Scale Methods in Dislocation Dynamics Simulations and Its Application in Work-Hardening

Author(s): Amin Aghaei, Ryan Sills, Wei Cai, *Stanford U.*.

Dislocation dynamics (DD) provides a systematic framework for the simulation of metal plasticity and strain hardening. DD models follow the motion of a network of dislocation lines discretized into segments and connected by a set of nodes, which are the degrees of freedom of the system. In order for DD simulations to provide insight into the strain hardening process, they must be able to reach plastic strains on the order of experimental values (>10%). Despite the development of massively parallel algorithms and codes, this level of plastic strain has been out of reach thus far. A major cause of this computational gap is inefficient time integration. In order to remove this limitation, we have developed advanced time integration algorithms for 3D DD simulations. We show that DD simulations contain unstable modes, which force explicit second-order time-integrators to take very small time steps, while higher-order time-integrators offer much better performance. Unfortunately, there also exist unstable and highly non-linear modes that require a very small time step even when an implicit or explicit higher-order integrator is used. A significant speed-up is then achieved by the sub-cycling algorithm, in which nodes involved in the unstable and non-linear modes are time-integrated with small time steps while the remaining nodes are integrated with larger time steps. The performance of these advanced algorithms in large-scale DD simulations is evaluated.

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Title: Goal-Oriented Sensitivity Analysis and Error Estimation for an Adaptive Mesh Refinement Moving Boundary Flow: Application on Geophysical Flow

Author(s): Hossein Aghakhani, Abani K. Patra, *U. Buffalo*.

Adjoint solutions are extensively used in many applications including dual weighted error estimation, optimization and sensitivity analysis. Since the derivation of the continuous adjoint is not possible for some operators due to the inadmissible boundary conditions, the discrete adjoint is the acceptable way of computing the adjoint. However, computing the adjoint of a nonlinear system of PDEs in a scalable code that benefited from grid adaptivity in an affordable way has been a challenge especially when the degrees of freedom are very large. Some of the difficulties that have to be handled are huge data I/O, allocating and deallocating memory for data structures, efficient data communication, finding appropriate interpolation and prolongation operators. These difficulties increase when the domain of the problem changes due to a moving boundary flow.\newline In this study, we investigated the effect of different parameters such as different data structures and simple but efficient interpolation and prolongation operators to firstly decrease the computational cost of the adjoint computation. We also showed how to overcome the difficulties arising from moving boundary flow. In the next part of the work, we used the adjoint solution to quantify the error in the functional of interest. Since we are interested in geophysical flows, and our final goal is to construct a hazard map for some location under the effect of a geophysical flow, we test different functionals in order to better understand extreme conditions like maximum height of the flow.

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Title: Pressure Transferable Coarse-Grained Potentials for Polyethylene

Author(s): Vipin Agrawal, Jay Oswald, *Arizona State U.*.

We present recent progress in coarse-grained simulations of polyethylene under shock loading. Coarse-grained models calibrated to match polymer structural properties generally lack representability of physical properties and transferability across thermodynamic states. We explore a new model that includes many-body interactions which are calibrated against MD simulations at various levels of isothermal compression, up to 15 GPa. Verification of this new model is established by comparing the predicted bulk modulus, shock Hugoniot P-v and us-up curves with atomistic MD calculations. More rigorous thermodynamic performance of the new coarse-grained model is investigated by computing the temperature rise along the Hugoniot through the Mie-Gruneisen equation of state. Lastly, the general applicability and potential shortcomings of this new CG model for prediction of thermodynamic properties of polymer systems will be discussed.

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Title: A Second-Order Accurate Mathematical Optimization Algorithm Fully Based on First-Order Information

Author(s): Miguel A. Aguilo, *Sandia Nat'l. Lab.*.

Mathematical optimization is encountered in many scientific and engineering fields. The task of optimizing a given function by finding the set of input parameters given a feasible set, i.e. constraint set, can be often daunting due to the complex nature of mathematical optimization problems. These problems often demand advanced mathematical optimization algorithms combined with second-order derivative operators to achieve quadratic convergence rates. However, deriving these second-order derivative operators can be a difficult task due to the expertise that is needed to derive and verify these derivative operators. This work presents a matrix-free mathematical optimization algorithm that employs first-order information to automatically derive second-order derivative information. The algorithm applies finite difference numerical integration techniques to derive the second-order derivative operators required to compute the application of the trial step to the Hessian operator. This feature enables the algorithm to achieve quadratic convergence rates at no additional computational cost, independent of the number of optimization parameters. The algorithm is further designed to not be specific to the numerical integration technique. This design enhances the algorithm's flexibility and robustness by facilitating the application of the optimal numerical integration technique, e.g. higher-order techniques, for a given problem. Finally, to ensure that the algorithm converges to an optimal and feasible solution, the algorithm is designed to use either line search or trust region methods. Examples in topology optimization will be presented to show the feasibility of the proposed mathematical optimization algorithm for this class of problems. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Reduced-Order Modeling of Turbulent Flows with Applications in Nuclear Reactor Components

Author(s): Mohammad Ahmadpoor, *U. Pittsbutgh*; Greg Banyay, John Brigham, *U. Pittsburgh*.

The overall objective of the current works is to explore approaches for computationally efficient reduced-order modeling (ROM) of non-isothermal turbulent mixing in high temperature reactors. The present focus is on turbulent flow past a cylinder in an open domain. Despite improvements in computing power and advancements in Computational Fluid Dynamics (CFD), the computational simulation of Navier-Stokes equations is still computationally expensive for the purpose of optimization and control of unsteady flows in even simple systems. Hence some form of accurate and realistic model reduction is necessary for enabling computational analysis to aid in design and control problems. In general, there are two fundamental steps to create a basis for a ROM: (1) acquisition of an ensemble of possible solution fields (e.g., distributions of flow or temperature that could potentially be seen in the system) for the system under consideration and (2) Extracting key features of the ensemble to create a basis (modes). Proper Orthogonal Decomposition (POD) is one approach for extracting features from an ensemble that provides the basis of the chosen dimension such that the average L2-error is minimized for the best approximation of the basis to the given ensemble. At present, POD is used to capture the parametric variation of unsteady flows. From the theoretical point of view, it is not clear how well POD modes, and the low dimensional models based on them, perform at Reynold's (Re) numbers different from the one at which they were constructed (The basis set is optimal for one Re number). To address the aforementioned question, the present work investigates the accuracy and efficiency of the ROM constructed from multiple Re numbers and also the long-term behavior of the ROM. Two approaches are numerically explored here for model reduction of turbulent flow past a cylinder: (1) a regression-based approach, which does not keep the mathematical structure of the modeling, but rather uses interpolation and/or extrapolation to predict flow fields at different Re number or different times and (2) a Galerkin-projection approach in which the Navier-Stokes equations are projected onto the POD modes to obtain low-dimensional ordinary differential equations to represent the fluid flow under conditions outside of the original ensemble. The computational expense and relative accuracy with respect to both extrapolation and interpolation in the Re number domain will be discussed.

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Title: A K-Profile Parameterization of Vertical Mixing Induced by Langmuir Turbulence in Shallow Water

Author(s): Nityanand Sinha, Andres E. Tejada-Martinez, *U. South Florida*; Cigdem Akan, *UC Los Angeles*.

Wave-current interaction gives rise to Langmuir turbulence characterized by Langmuir circulation (LC) consisting of a spectrum of scales of counter rotating vortices roughly aligned in the direction of the wind. Large-eddy simulations (LES) of LC in a wind-driven shear current have shown that vertical mixing due to the LC disrupts the classical bottom log layer velocity profile generating a wake region instead. Near the surface, Stokes drift shear (responsible for generating LC) serves to intensify small scale eddies leading to enhanced mixing and disruption of the surface velocity log-law. Analysis of Reynolds shear stress budgets reveals that LC also induces negative mean velocity shear under certain combinations of wind and wave forcing parameters leading to nonlocal transport. We present a K-profile parameterization (KPP) comprised of local and nonlocal components which can represent these vertical mixing mechanisms by which Langmuir turbulence impacts the mean flow. Good agreement in terms of mean velocity was found between LES and single water column RANS (Reynolds-averaged Navier-Stokes) simulations with the new KPP.

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Title: Towards a Fully Implicit Level-Set Approach for Free-Surface Problems

Author(s): Ido Akkerman, *TU Delft*.

We present a fully implicit level-set approach. The level-set is used to split the domain in separate air and water domains. Due to the sharp interface there is no need for redistancing. Redistancing is highly non-linear process that is often costly and hard to do robustly, so it is essential to avoid when aiming for a fully implicit approach. In order to correct the mass error prevalent in level-set methods we add a global correction to the level-set as reported in [1]. The method of splitting the domain in distinct domains is relatively straight forward for meshes consisting of solely tetrahedral elements. In this case the elements get subdivided in either 2 prismatic elements or a prismatic and a tetrahedral element. As these prismatic elements have nonlinear mappings, a highly accurate integration scheme is essential. In the future we plan to extend the method to rigid bodies [2] and elastic bodies. In fact the attempt to extend the approach reported in [2] with elastic modes is what initiated the shift to fully implicit methods as we ere not able to device a staggered approach that worked. Additionally, the fully implicit approach should facilitate obtaining a (globally) mass, momentum and energy conservative integration scheme. [1] Kees C, Akkerman I, Farthing M, Bazilevs Y (2011) A conservative level set method suitable for variable-order approximations and unstructured meshes. J Comput Phys 230(12):3402–3414 [2] Akkerman I, Bazilevs Y, Benson DJ, Farthing CE, Kees MW (2012) Free-surface flow and object interaction modeling with emphasis on ship hydrodynamics. J Appl Mech 79(1):010909

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Atomic Scale Exploration of Stress Manifestation During Metallic Film Growth

Author(s): Murat Al, *Lehigh U.*.

This study will elucidate stress manifestation during atomic scale processes associated with metallic film growth. When separate regions of growing film approach one another, coalescence events occur that close gaps between them; this is driven by a reduction in surface energy, but it occurs at the cost of an increase in elastic (tensile) energy. While much has been revealed via experiments that measure film stress during growth, these studies typically present data for the total film stress. Less is known about the distribution of stress in a film for which a given value of total stress is quoted. To study such phenomena, coalescence processes in monolayer films of Au on Ni (001) substrates were modeled with molecular dynamics (MD) simulations at 300K. The Au/Ni binary was selected because this system exhibits significant lattice mismatch and a positive heat of mixing, allowing examination of the effect of epitaxial mismatch but with a sharp interface between film and substrate. Model deposition produced Au monolayer films of (111) hexagonal character. To model coalescence, a defect was introduced by deletion of Au atoms in a line along one of the periodic dimensions in the plane of the film. Subsequent simulations allowed model films to coalesce; stress distribution in the film was computed as a function of time over simulations spanning of order one microsecond. The effect of model monolayer size was studied by varying both in-plane film dimensions. The y-direction was perpendicular to the line defect and x was parallel; thus, Ly was the distance between line defects in a model of a periodically defected infinite monolayer. For Ly = 3 nm, a relatively uniform stress was computed in the film; for Ly = 6 nm and larger, stress localization near the coalescence region was observed with stress distributions reaching a peak at the coalesced defect and decaying down to near zero stress sufficiently far from the defected area. The width of the region with non-negligible stress manifestation (~3 nm) was relatively insensitive to either Lx or Ly; however, the peak stress decreased with increasing Lx. The same was true for Ly but to a lesser degree. A thermodynamic limit analysis was performed for peak coalescence stress. Stress as computed via both the standard virial expression as well as via methods due to Hardy will be presented; while the magnitude of peak stress was dependent upon the method employed, stress localization width was not.

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Title: Isogeometric Analysis Suitable Trivariate NURBS Models from Standard B-Rep CAD

Author(s): Hassan Al Akhras, Thomas Elguedj, Anthony Gravouil, *U. Lyon*; Michel Rochette, *ANSYS* .

We present an automatic algorithm for constructing a volumetric NURBS parameterization from boundary representation CAD models. The starting point of our algorithm is a triangulated surface bounding a solid region. Our algorithm pipeline includes four main steps: - Pants decomposition of the boundary surface. Such segmentation decomposes a complicated surface into a set of shapes that have a trivial topology (genus-0 surface with 3 boundaries). - Decomposing of each pants patch into a set of cuboid patches using a parameterization based on the generalized Koebe's method. Each cuboid is one boxed region enclosed by 6 disk-like surface patches. - Mapping each cuboid to the surface of a unit cube in the parametric domain by applying the harmonic parameterization method. Based on this parameterization, 6 compatible and valid B-spline boundary surfaces are reconstructed. - Computing the interior volumetric parametrization by using the B-spline surfaces as boundary conditions. The volumetric NURBS mesh can be then used for isogeometric analysis. The efficiency and the robustness of the proposed approach will be illustrated by several examples.

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Title: Multi-Dimensional Precipitation Patterns and the Cahn-Hilliard Reaction-Diffusion Equations

Author(s): Mazen Al-Ghoul, *American U. Beirut*.

The use of reaction-diffusion mechanism at the micro- and nono-scales has recently picked a considerable momentum in materials science to fabricate a variety of small-scale structures such as micro-lenses, complex microfluidic architectures, optical elements, chemical sensors and amplifiers, etc. [1] Therefore the need of working models is complementary the to the aforementioned experimental endeavors. In this work, we present new emerging 2D and 3D precipitation patterns that can be used as templates to fabricate complex microstructures and we will present a model that is based on a phase separation scenario of colloidal particles that are first produced by the chemical reaction [2]. Under suitable conditions, these colloidal particles could subsequently phase separate into regions of low concentration (no precipitate) and high concentration (precipitate) leading to precipitation patterns. We show that such dynamics can be described by a nonlinear Cahn-Hilliard (CH) equation for the colloid coupled to reaction-diffusion equations of the initial reactants [1]. The resulting equations will be solved using an Isogeometric Analysis [2] and a generalized-α time adaptive scheme. We demonstrate that our model and multi-dimensional solutions are capable of describing the complex dynamics and emerging patterns. [1] M. Dayeh, M. Ammar, and M. Al-Ghoul, Transition from rings to spots in a precipitation reaction-diffusion system, RSC Adv., 4 (2014), pp. 60034–60038. [2] H. Gómez, V. M. Calo, Y. Bazilevs, and T. J. R. Hughes, Isogeometric analysis of the Cahn-Hilliard phase-field model, Computer Methods in Applied Mechanics and Engineering, 197 (2008), pp. 4333–4352.

13th U.S. National Congress on Computational Mechanics
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Title: Connecting Mimetic Finite Differences and Finite Volume Methods for Voronoi Diagrams

Author(s): Omar Al-Hinai, Mary F. Wheeler, *UT Austin*; Ivan Yotov, *U. Pittsburgh*.

There has been a known connection between Finite Volume methods (FVM) and Mixed Finite Elements (MFE). However, classical MFE cannot be easily extended to certain FVM in cases of general polyhedra. One example is the case of Voronoi diagrams, which permit a certain class of robust FVM techniques. The Mimetic Finite Difference method (MFD) is in the same family as MFE and works over very general polyderal elements. In this work, we demonstrate a generalization of MFD that establishes a connection with these classical FVM over Voronoi diagram. Establishing such a connection extends theoretical results from MFD to FVM. In addition, it provides for opportunities to reduce computational and memory overhead of the MFD method. In addition, the proposed generalization extends the cases for which MFD discretizations satisfy the maximum principle. We present first order convergence results for the scalar and vector unknowns. In addition, we present second order (superconvergence) results for the scalar variable under certain restrictions. This is accompanied by novel lifting operators for the square element. We discuss the application of these ideas to porous media flow applications with an emphasis on complex fracture modeling.

13th U.S. National Congress on Computational Mechanics
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Title: A Non-Linear Simplified FSI-Model: Application to Autoregulated Flows

Author(s): Matteo Aletti, Jean-Frédéric Gerbeau, Damiano Lombardi, *Sorbonne U., UPMC U. Paris* .

Fluid-Structure Interaction (FSI) plays an important role in blood vessels networks. The full-order FSI simulation is costly from a computational point of view, making large scale systems prohibitive to simulate. To reduce the computational cost, simplified FSI numerical methods were proposed. The main idea, which is exploited also in the present work, is to embed the effects of the structure into the fluid equations by defining an hybrid Dirichlet-Robin boundary condition. At each time step, only the fluid equations are solved. A fixed mesh discretisation with first-order transpiration conditions is adopted, to avoid the use of an ALE formulation. The structure dynamics is described by a two-layer model: a simplified non-linear Koiter shell model and a non-isotropic fiber layer. We assume that the wall displacement is aligned with the normal unit vector to the reference configuration and that bending terms are negligible, while the fibers constitutive law is that of an elastic linear pre-stressed spring. Several synthetic testcases are proposed to validate this approach and compare its performances to other works in the literature. The application that motivated this work is the description of autoregulation in the cardiovascular system. Autoregulation is a key phenomenon in the modeling of blood flow in the micro-circulation regime: micro-vessels are able to maintain an approximately constant flow rate despite changes in the incoming pressure and also to regulate the flow rate accordingly to metabolic needs. The vessels wall is characterized mainly by two layers: a thin endothelium layer and a particularly developed layer of smooth muscle cells that are able to contract or to relax in order to change the vessel diameter and then its resistance. Simulations of autoregulated flows are shown, in geometries based on medical images, with a pressure non-linear feedback control. This research was made possible by a Marie Curie grant from the European Commission in the framework of the REVAMMAD ITN (Initial Training Research network), Project number 316990. An Effective Fluid-Structure Interaction Formulation for Vascular Dynamics by Generalized Robin Conditions F. Nobile and C. Vergara SIAM Journal on Scientific Computing 2008 30:2, 731-763 A coupled momentum method for modeling blood flow in three-dimensional deformable arteries Figueroa, C. Alberto, et al Computer methods in applied mechanics and engineering 195.41 (2006): 5685-5706. Pressure Boundary Conditions for Blood Flows. Kirill Gostaf, Olivier Pironneau. <hal-00865671> 2013.

13th U.S. National Congress on Computational Mechanics
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Title: Minimization of Sonic Boom Using Adjoint Technique

Author(s): Navid Allahverdi, *NYC College of Tech*; Alejandro Pozo, Enrique Zuazua, *BCAM*.

Sonic boom is generated due to supersonic flights of planes and it is perceived as two loud bangs on the ground. Sonic boom causes annoyance for human hearing. The realization of supersonic commercial air travel is contingent on lowering the intensity of sonic boom perceived on the ground. In this talk, different aspects of modeling sonic boon propagation in the atmosphere and approaches to minimizing the intensity of the sonic boom on the ground will be presented. The propagation of sonic boom in the atmosphere is modeled by means of augmented Burgers equation (ABE), which is a nonlocal version of the viscous Burgers equation used in nonlinear acoustics. The augmented Burgers equation takes into account nonlinear effects, such as waveform steepening and variable-speed wave propagation, as well as molecular relaxation phenomena, ray tube spreading and atmospheric stratification. The ABE is solved via operator splitting techniques. It takes a long time for the sonic boom to reach the ground in comparison with the time scale of the pressure signal. This fact necessitates using conservative fluxes in discretizing and integrating ABE in the long time horizon. The sonic boom minimization is formulated as an optimal control problem where initial condition to ABE serves as the control, and the objective functional measures the distance between ground pressure and a target signature in a suitable norm. At the optimization level, an adjoint methodology based on optimize-then-discretize approach is used to obtain the minimizers. The adjoint equation is solved using an operator splitting approach. In this talk, the results obtained for direct problem and inverse problem will be presented. Major drawbacks in using adjoint technique as well as remedies to the limitations will be discussed. The major drawbacks include lack of sensitivity of objective functional to high frequency modes, as well as, the biased nature of the adjoint methodology in recovering smooth initial solutions. Employing proper norms will alleviate the insensitivity of the objective functional to high frequency modes.

13th U.S. National Congress on Computational Mechanics
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Title: Finding All Roots of Fuzzy Polynomials

Author(s): Ibraheem Alolyan, *King Saud U.*.

In this paper, we find the real roots of Interval quadratic polynomials, where all the coefficients are intervals. A method to compute the interval roots is developed. The characterization of the roots of the interval polynomials is obtained as a function of their interval coefficients adequately defining certain polynomials with real coefficients.

13th U.S. National Congress on Computational Mechanics
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Title: Non-Linear Waves of Viscoelastic Liquid Curved Jets in the Giesekus Model

Author(s): Abdullah Alsharif, *Taif U.*.

The industrial prilling process has many applications in engineering and manufactures ,such as sprays ,fertilizers ,ink jets printing and roll coating. This prilling process is used to produce droplets, which are generated from breaking up the liquid jets (when the liquid emerges from the orifices of the prilling process). Most of the liquid, which are used in this process, is mixture of various fluids. Therefore we consider the liquid as a non-Newtonian fluid and the viscoelastic nature by using the Giesekus model. In addition, we assume that a large cylindrical drum, which has a radius s, and rotates with angular velocity Ω. There is an orifice , has a radius a, on the side of this drum to allow the liquid to emerge and then to break up into small droplets. These droplets solidify to the form pellets. The jet is curved in the space due to the rotation and gravity. In order to understand the mechanism of the jet break-up in the prilling process, we consider a mathematical modeling to capture the essential physics related to a cylindrical drum (see Alsharif etal., instability of viscoelastic curved jets, Appl. Math. Modell. (2015). We use the asymptotic analysis to reduce the governing equations into 1-D equations. Furthermore, the steady state solutions have been found by using the Range-Kutta method. In the linear theory, we cannot give a good prediction of the break-up and the droplet sizes of the prilling process. Thus we have used a finite difference scheme based on the Lax-Wendroff method to determine the break-up lengths and main and satellite droplets, because this phenomenon is nonlinear. We have found from our results that decreasing the Reynolds number, which corresponds to high viscosity, increases break-up length. It is also found that increasing the viscosity ratio (the total of the solvent and polymeric liquid) leads to an increase in the break-up length. Moreover, we observed that satellite droplet sizes decrease when the Rossby number, Rb, is decreased (meaning the rotation rates decreases), whereas main droplet sizes remain steady. We also noticed that increasing the mobility factor leads to an increase in the break-up lengths of the viscoelastic jet.

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Title: Modelling Cancellous Bone: An Elastic Mixture Theory Approach

Author(s): S Burhanettin Altan, *Bayburt U.*; Turgut Göksoy, *Regional Hospital*.

Bones are common in all mammals which are typical examples of open cell porous media that can be found in the nature as light-weight structural elements. Open cell porous media are also used as materials for light-weight structural elements with high specific strengths as well as thermal insulators. It is an ongoing active research field to develop methods to predict the mechanical behavior of open cell porous media. Open cell porous media can be envisioned as a collection of randomly interconnected struts. The properties, both the geometrical (cross- sectional area and length) and the mechanical (Young's modulus, Poisson ratio, fracture) ones of the struts may exhibit significant variations from cell to cell, even within a cell. The complexity of the structure of the open cell porous media poses difficulty for modelling their mechanical behavior. Finite Element Analysis (FEA) has been proven to be useful to model the mechanical behavior of open cell porous media. Li et al. [1] studied the mechanical response of an open cell porous medium with various cell size and strut cross sectional area. Another approach for modelling the mechanical behavior of porous medium is to replace it with an equivalent continuum for which Gibson and Ashby [2] can be referred to. A homogenization method for modelling mechanical behavior of cancellous bone employing the theory of elastic mixtures is introduced. A short survey on cancellous bones and importance of its mechanical behavior is provided. The models available in the literature for the mechanical behavior of cancellous bones are summarized. The scheme for modelling the solid skeleton of cancellous bone is introduced in full detail. Wave propagation in cancellous bone is studied and it is shown that the constitutive equation obtained in the study is capable to represent positive and negative dispersion as well as attenuation. The effect of bone marrow on wave propagation is discussed by incorporating a generalized Biot's theory. This study is concluded by indicating that the quantitative ultrasound can be extended to obtain some estimation about the micro-architectural parameters of cancellous bone. REFERENCES [1] Li, K., X. L. Gao, et al.. "Effects of Cell Shape and Strut Cross-Sectional Area Variations on the Elastic Properties of Three-Dimensional Open-Cell Foams", Journal of the Mechanics and Physics of Solids, 54(4): 783-806, 2006. [2] Gibson, L. J., M. F. Ashby Cellular Solids: Structure and Properties, Cambridge University Press, 1999.

13th U.S. National Congress on Computational Mechanics
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Title: Advances in Error Estimation for Homogenisation

Author(s): Daniel Alves Paladim, Pierre Kerfriden, *Cardiff U.*; José Paulo Moitinho de Almeida, *U. Lisboa*; Mathilde Chevreuil, *U. Nantes*; Stéphane Bordas, *Luxembourg U.*.

In this paper, the concept of modeling error is extended to the homogenisation of elliptic PDEs. The main difficulty is the lack of a full description of the diffusion coefficients. We overcome this obstacle by representing them as a random a field. Under this framework, it is possible to quantify the accuracy of the surrogate model (the homogenised model) in terms of first moments of the energy norm and quantities of interest. This work builds on the seminal work of [1]. The methodology here presented rely on the Constitutive Relation Error (CRE) which states that a certain measures of the primal and dual surrogate model upper bound the exact error. The surrogate model, in agreement with homogenisation, is deterministic. This property exploited to obtain bounds whose computation is also deterministic. It is also shown that minimising the CRE in the set of homogenisation schemes leads us to an optimal surrogate that is closely related to the classical Voigt and Reuss models. Numerical examples demonstrate that the bounds are easy and affordable to compute, and useful as long as the mismatch between the diffusion coefficients of the microstructure remain small. In the case of high mismatch, extensions are proposed, through the introduction of stochastic surrogate models. [1]Romkes, Albert, J. Tinsley Oden, and Kumar Vemaganti. "Multi-scale goal-oriented adaptive modeling of random heterogeneous materials." Mechanics of materials 38.8 (2006): 859-872.

13th U.S. National Congress on Computational Mechanics
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Title: Topology Design of Antenna Applied to the Treatment of Cancer by Hyperthermia

Author(s): Alan Amad, Thiago Quinelato, Abimael Loula, Antonio Novotny, *LNCC/MCTI*.

Hyperthermia therapy is a non-invasive medical treatment in which body tissue is artificially heated through electromagnetic waves, focusing the heat in cancerous cells undergoing apoptosis. The regional electromagnetic hyperthermia problem is modeled by a semi-coupled system of partial differential equations. The heat equation in biologic tissues, or bioheat equation, is coupled with the Helmholtz equation. Electromagnetic waves are generated by spatially distributed antenna. This antenna produces a source in the Helmholtz equation, which solution appears as a heat source in the bioheat equation. Therefore, the basic idea consists in finding a distribution of heat source generated by electromagnetic antenna, which is able to focus the heat into the tumor while keeping the temperature under control in the healthy tissue. In particular, we are interested in the design of the support of the antenna, which leads to a topology optimization problem. There are many methods that could deal with such a problem like SIMP (Solid Isotropic Material with Penalisation) and level-set, for instance. However, in this work we propose a new optimization method based on the topological derivative concept to find the optimum configuration for the antenna. The topological derivative is, conceptually, a derivative of a shape functional with respect to infinitesimal changes in its topology, such as adding an infinitesimal hole, inclusions, source-terms or crack. The topological derivative has been proved to be useful in many relevant applications such as topology optimization, inverse problems, image processing, multi-scale constitutive modeling, fracture mechanics and damage evolution modeling. Finally, numerical experiments are presented, showing that the antenna obtained via the proposed topology optimization methodology are able to selectively heat the target and illustrating a possible application to cancer treatment by hyperthermia. In addition to the new optimization method, we are proposing a novel hybrid finite element formulation, both for the Helmholtz problem and the heat problem. L. Wu, R. J. McGough, O. A. Arabe, T. V. Samulski, An RF phased array applicator designed for hyperthermia breast cancer treatments, Physics in Medicine and Biology 51 (1) (2006) 1–20. A. A. Novotny, J. Sokolowski, Topological derivatives in shape optimization, Interaction of Mechanics and Mathematics, Springer, 2013.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Topology Optimization Procedures with Material Nonlinearities for Reducing Stress Concentrations

Author(s): Oded Amir, *Technion*.

One of the most important aspects of a viable topology optimization procedure is the capability to avoid stress concentrations in the optimized design. This can be achieved by considering stress constraints in the computational procedure. The local nature of stress constraints poses a significant difficulty: The corresponding optimization problem involves a large number of design variables as well as a large number of constraints. In this paper, we suggest an alternative approach in which the nonlinear, inelastic material behavior plays a central role. The optimization procedure drives the design towards a linear-elastic response by minimizing certain measures related to the inelastic part of the response. This implies that stress limits can be implicitly satisfied, without imposing a large number of local constraints. The objective in the proposed formulation is to minimize the sum of equivalent plastic strains over the whole design domain. The equivalent plastic strains are state variables determined from the elasto-plastic response governed by J2-flow theory. General constraints can be imposed on volume of material and on compliance, for a given prescribed displacement. Sensitivity analysis is formulated using the adjoint method, leading to a backwards-incremental procedure due to path-dependency of the primal analysis. Preliminary numerical experiments present promising results. For the classical case of an L-bracket, results obtained by the proposed approach resemble those obtained by other investigators who applied linear-elastic topology optimization procedures with either local or aggregated stress constraints (e.g. [1] and various references therein). The suggested procedure relies on nonlinear finite element analysis, meaning that it is more demanding in the analysis phase in comparison with existing approaches. Nevertheless, this added complexity is counter-balanced by the reduced complexity of the optimization problem, which involves only a few global constraints. Therefore, the proposed approach can be very attractive for large-scale scenarios. Furthermore, in comparison with constraint aggregation approaches, in the current approach all stress violations are captured accurately and can be reduced simultaneously due to the inclusion of plastic strains in the objective. These arguments and further considerations will be discussed in detail. [1] C. Le, J. Norato, T. Bruns, C. Ha, D. Tortorelli. Stress-based topology optimization for continua, Structural and Multidisciplinary Optimization, 41(4), 605-620, 2010.

13th U.S. National Congress on Computational Mechanics
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Title: Real-Time PDE-Constrained Optimization Using Databases of Parameterized Reduced-Order Models

Author(s): David Amsallem, Youngsoo Choi, Radek Tezaur, Charbel Farhat, *Stanford U.*.

A comprehensive framework for the fast solution of PDE-constrained optimization problems is presented. The approach relies on three key components 1) the development of reduced-order modeling techniques for the fast solution of the PDE at a given configuration, 2) the generation of databases of such parameterized reduced models and 3) interpolation procedures to compute on-the-fly solutions of reduced-order models at novel configurations in the optimization phase. Greedy parameter sampling techniques are developed to minimally generate and train the database in an offline phase prior to its use in the online phase to solve the optimization problem of interest. The proposed framework will be illustrated by its application to the aeroelastic design optimization of a realistic wing structure as well as the solution of inverse problems in acoustic scattering.

13th U.S. National Congress on Computational Mechanics
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Title: Stokes-Cahn-Hilliard Formulations and Simulations of Two-Phase Flows with Suspended Rigid Particles

Author(s): Patrick Anderson, Nick Jaensson, Martien Hulsen, *Eindhoven U. Tech.*.

Three formulations of the Stokes-Cahn-Hilliard (SCH) system are investigated for the simulation of rigid particles in two-phase flows. Using the SCH framework, we assume that the interface between the two fluids is diffuse, whereas the interface between the fluids and the particle is assumed to be sharp. To describe the sharp boundary of the particle, a moving, boundary-fitted mesh is used which is refined near the fluid-fluid interface. The three formulations, the “stress form” and two “potential forms”, are first investigated in the absence of traction boundary conditions, by simulating a retracting droplet in a closed, cylindrical container. We show that the three formulations perform similar in terms of accuracy, although the velocity is slightly more accurate for the potential forms. When investigating mesh-convergence, superconvergence of the velocity and chemical potential is observed in the three forms. In equilibrium, the stress form shows higher parasitic currents near the interface. When comparing the pressure as it is defined in the stress form, the potential forms show higher peaks in the pressure near the interface. The three methods are stable when simulating a stationary droplet for a long period of time. For the potential forms, an additional integral term arises on the particle boundary. When investigating mesh- convergence, we observe superconvergence of the location and velocity of the particle, the velocity field and the chemical potential if the stress form is used. However, subconvergence is observed for these variables when using the potential forms. The three methods are stable when simulating a particle that is captured at a fluid-fluid interface for a long period of time.

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Title: Hilbert Complexes and Finite Element Spaces for Second-Order Tensors

Author(s): Arzhang Angoshtari, Arash Yavari, *Georgia Inst. Tech.*.

We introduce some finite elements for second-order tensors by using suitable Hilbert complexes and the finite element exterior calculus. These elements can be considered as the tensorial analogues of some standard finite elements for vector fields. An important feature of these elements is that they respect the global topology of domains in the sense that they can reproduce certain topological properties of domains. We obtain stable mixed finite element methods for the tensor Laplacian by means of these elements. A potential application of these elements is developing mixed finite element methods for nonlinear elasticity on domains with irregular geometries.

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Title: A Phantom-Node Approach for Modeling Complex Fracture Networks

Author(s): Chandrasekhar Annavarapu, Efrem Vitali, Randolph Settgast, *LLNL*.

The phantom node approach was originally introduced by Hansbo and Hansbo [1] to model strong and weak discontinuities in solid mechanics. The equivalence of the phantom node formulation and the eXtended Finite Element Method (XFEM) was shown in [2]. However, unlike the XFEM, the phantom node approach lends itself to be readily adapted in an already existing finite element package and has hence become increasingly popular. While the approach has been extended to many diverse application areas including dynamic crack and shear band propagation, fluid-structure interaction and micro-structural materials, relatively few studies have focused on the important problem of intersecting interfaces ([3], [4]). We present a method that extends the phantom-node approach to the case of complex fracture networks including multiple intersecting fractures and fracture tips. We discuss a hierarchical framework for altering the background mesh-topology in the presence of many intersecting fractures. Finally, we assess the numerical performance of the method through several benchmark numerical examples in 2D. References: [1] Hansbo, P. and Hansbo A., A finite element method for the simulation of strong and weak discontinuities in solid mechanics, Comput. Meth. Appl. Mech. Engrg., 193(33-35):3523– 3540, 2004. [2] Song, J-H., Areias P. and Belytschko, T., A method for dynamic crack and shear band propagation with phantom nodes, Int. J. Num. Meth. Engrg., 67: 868–893, 2006. [3] Richardson, C. L., Hegemann, J., Sifakis, E., Hellrung, J. and Teran, J. M., An XFEM method for modeling geometrically elaborate crack propagation in brittle materials. Int. J. Numer. Meth. Engrg., 88: 1042–1065, 2011. [4] Annavarapu, C., Hautefeuille, M. and Dolbow, J. E., A Nitsche stabilized finite element method for frictional sliding on embedded interfaces. Part II: Intersecting interfaces, Comput. Meth. Appl. Mech. Engrg., 267(1): 318–341, 2013.

13th U.S. National Congress on Computational Mechanics
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Title: Large-Scale Suspension Flow Simulations Using a Particle Method on a GPU Supercomputer

Author(s): Takayuki Aoki, Satori Tsuzuki, Seiya Eatanabe, *Tokyo Inst. Tech.*.

It is one of challenging topics to carry out large-scale SPH simulations. Current supercomputers consist of multiple nodes and each node of Tokyo Tech supercomputer TSUBAME2.5 has three GPUs (Graphics Processing Unit) and there are 1,403 nodes in the total system. SPH simulations have to run efficiently on the memory-distributed systems. Particles used in the SPH simulation can move randomly in the computational domain. The particles are divided into the subdomain keeping the same number particles by a dynamic domain decomposition to have an equal load balance. We introduce the slice-grid method in which the vertical boundaries of the subdomains move first to keep the vertical load balance of the horizontal subdomain group and the horizontal boundaries of the subdomains move individually next. The particles across the subdomain boundaries are transferred to the neighbor subdomains through the interconnection network. This causes memory fragmentation and we execute a de-fragmentation with a proper frequency. A linked-list algorithm for the neighbour particle list is also introduced to reduce the memory use drastically. We succeeded in carrying out a large-scale SPH simulation with the maximum 1.0 billion particles for a suspension flow including 2,304 cubic objects were conducted by using 87.4 million particles on 256 GPUs.

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Title: A Novel Chemo-Mechano-Biological Mathematical Model of Arterial Tissue Growth and Remodeling: Modelling of Signaling Pathways Governing Adventitial Adaptive Response

Author(s): Pedro Aparicio, Mark Thompson, *U. Oxford*; Thomas Rahman, *U. Sheffield*; Paul Watton, *U. Sheffield*.

A novel Chemo-Mechano-Biological (CMB) mathematical model of arterial wall growth and remodeling (G&R) is proposed. The artery is modelled as a nonlinear elastic cylindrical membrane (Watton et al, 2009) and two important classes of stimuli influencing vascular cellular response are represented: (a) mechanical stimuli; and (b) levels of cellular and biochemical species mediating arterial extracellular matrix G&R. In particular, a model of the Transforming Growth Factor (TGF)-beta profibrotic signaling pathway (Dale et al, 1996) was adapted and extended to capture the role of this signaling peptide as a mechanotransduction mediator signaling adventitial fibroblasts to upregulating matrix deposition. The model is further enriched by incorporating biologically-inspired laws governing the evolution of the collagen fibre attachment stretch distribution. The model is applied to simulate the development of inflammatory arterial aneurysms. The adventitia is initially modelled as a protective sheath. As the aneurysm develops, the adventitial collagen attachment stretch distribution evolves so that the adventitia plays a load bearing role. The TGF-beta signaling pathway is numerically explored by prescribing different rates of TGF-beta production as a result of deviation from mechanobiological homeostasis following initial partial matrix degradation. The model predicts that slower mechanotransduction leads to faster growing aneurysms. Application of a “therapeutic” step increase in TGF-beta leads to transient arrest of growth and later domain stabilization at lower stretches; this is consistent with experimental observations suggesting a protective role of TGF-beta against inflammatory aneurysm expansion, e.g. (Dai et al, 2005). We conclude that this novel model provides an in silico test bed for exploring chemo-mechano-biological mechanistic hypotheses to further our understanding of vascular homeostasis and disease. References: Dai, J., et al. (2005) Overexpression of Transforming Growth Factor-beta1 Stabilizes Already-Formed Aortic Aneurysms. Circulation. 112:1008-1015 Dale, P.D., et al. (1996) A mathematical model for collagen fibre formation during foetal and adult dermal wound healing. Proc. R. Soc. Lond. B. 263: 653-660. Watton, P.N., et al. (2009) Modelling the growth and stabilization of cerebral aneurysms. Mathematical Medicine and Biology. 26:133-164.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Analytical and Numerical Studies on the Modified Error in Constitutive Equations Approach for Inverse Elastodynamics

Author(s): Wilkins Aquino, *Duke U.*; Marc Bonnet, *ENSTA*.

The Modified Error in Constitutive Equations (MECE) has been gaining more attention in recent years due to some of its inherent advantages such as strong physical meaning of the objective functional, robustness with respect to initial guess and noise, and insensitivity to resonances, among others. The MECE approach departs from conventional PDE-constrained formalisms in that an error in constitutive equations functional appears as part of the objective to be minimized. Furthermore, as opposed to conventional approaches, the PDE constraint involves just fundamental conservation laws without including the constitutive relations that connect fluxes (e.g. stresses) and gradients of state variables (e.g. strains). In this fashion, the constitutive relation is relaxed, as it appears in a penalty-like form in the objective functional. In this work, we present analytical results that support some of the advantages of MECE approaches that have been reported recently. Specifically, we put forward conditions for well-posedness and convergence of FE discretizations of the coupled variational problems that appear as part the KKT system. Moreover, we demonstrate that conventional Error in Constitutive Equations (ECE) and Least Squares formulations are particular limiting cases of MECE formulations. In addition, we show the sense in which the weight parameter that appears in the MECE approach serves as a regularizer. Our theoretical results are demonstrated through several numerical examples drawn from elasticity imaging applications.

13th U.S. National Congress on Computational Mechanics
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Title: A New Formulation for Imposing Dirichlet Boundary Conditions on Non-Matching Meshes

Author(s): Aurelia Cuba-Ramos, Jean-François Molinari, *EPF. de Lausanne*; Alejandro M. Aragón, *TU Delft*; Soheil Soghrati, *Ohio State U.*; Philippe H. Geubelle, *U. Illinois* .

Generating matching meshes for problems with complex boundaries is often an intricate process, and the use of non-matching meshes appears as an appealing solution. Yet, enforcing boundary conditions on non-matching meshes is not a straightforward process, especially when prescribing those of Dirichlet type. By combining a generalized finite element formulation (IGFEM) with the Lagrange multiplier method, a new method for the treatment of essential boundary conditions on non-matching meshes is presented. The new formulation yields a symmetric stiffness matrix and is straightforward to implement. As a result, the methodology makes possible the analysis of problems with the use of simple structured meshes, irrespective of the problem domain boundary. Through the solution of linear elastic problems, we show that the optimal rate of convergence is preserved for piecewise linear finite elements. Yet, the formulation is general and thus it can be extended to other elliptic boundary value problems.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Correlating the Free-Volume Evolution to Plastic Deformation of Highly Cross-Linked Polymers from Large-Scale, Coarse-Grained MD Simulations

Author(s): Amin Aramoon, *John Hopkins U.*.

Highly cross-linked polymer networks (e.g. epoxies) are widely used in many automotive, marine, and aerospace applications. Predicting the damage and failure of such systems is of crucial interest for the reliable performance of these class of materials. The evolving free volume (voids) in these networks under loading plays a critical role in both their elastic and plastic response. Macroscopic properties such as elasticity, glass transition temperature, and failure can be experimentally determined. In addition, the distribution and size of free volumes can be measured using positron annihilation techniques. However, in such studies it is not always easy to identify the microstructural features controlling plasticity and failure. On the other hand, numerical methods such as quantum mechanics (QM) and molecular dynamics (MD) simulations can shed light on the atomic processes involved, but are computationally expensive and limited to modeling extremely small volumes, and further linking the outcome of these methods with continuum models still requires further developments. In this work, a MD coarse-grain model has been developed to study the plastic behavior of DGEBA. A detailed atomic monomer is coarsened using Quantum Mechanics simulations to create tailored plastic behavior of DGEBA for this study. The cross-linked polymer network is created curing a dynamic cross-linking algorithm in different conditions such as temperature, cross-linker functionality and degree of cross linking. The effect of chain size, and degree of cross-linking are also investigated on the evolution of the free volume density and subsequently plastic deformation (e.g. hardening and failure). A novel algorithm is developed which find free areas between chains in the epoxy network. Free volumes are quantified by fitting the largest ellipsoids in the free areas between the chains in the network. From these simulations we also develop a strong correlation between the evolution of plastic deformation and the free volume density of the epoxy.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Enhancement of Ultrasound Images Using a Selective Average Filter and an Artificial Life Model

Author(s): Alex Araujo, *U. Federal de Mato Grosso do Sul*; Christos Constantinou, *Stanford U.*; João Tavares, *U. Porto*.

Nowadays, the computational processing of images is a field of huge research with many applications in several areas like, for example, in medicine as to noise removal [1], image enhancement [2] and segmentation [3]. Particularly in medicine, the images acquired in order to assist the diagnosis and the definition of appropriate treatment plans. In this study, we combine techniques of image filtering and enhancement in order to improve ultrasound images and facilitate their segmentation. The image filtering intends to reduce the speckle noise presented in the original images and is accomplished by applying a selective average filter [1]. After the image filtering, the enhancement of the smoothed images is performed using an artificial life model [2]. In order to study the effect that the approach proposed has on the segmentation of the processed images, 770 frames of ultrasound images of the female pelvic cavity, especially of the bladder and urethra, were preprocessed and then segmented using the algorithm proposed by Chan and Vese [3]. A comparison was performed between the segmentation results obtained from the original images and the ones from the processed images, which confirmed that the proposed approach is promising as led to borders more appropriate for the structures under study and fewer occurrences of over-segmentation. Acknowledgments This work is funded by European Regional Development Funds (ERDF), through the Operational Programme ‘Thematic Factors of Competitiveness’ (COMPETE), and Portuguese Funds, through the Fundação para a Ciência e a Tecnologia (FCT), under the project: FCOMP-01-0124-FEDER-028160/PTDC/BBB- BMD/3088/2012. The first author also thanks FCT for the PhD grant: SFRH/BD/61983/2009. References [1] A. F. de Araujo, J. M. R. S. Tavares, and C. E. Constantinou, “A selective denoising method to remove speckle noise,” in Computational Vision and Medical Image Processing IV - VIPIMAGE 2013, 111-113, 2013. [2] A. F. de Araujo, C. E. Constantinou, and J. M. R. Tavares, “New artificial life model for image enhancement,” Expert Systems with Applications 41(13):5892-5906, 2014. [3] T. Chan and L. Vese, “Active contours without edges,” Image Processing, IEEE Transactions on 10(2): 266-277, 2001.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Local Level Set-Based Approach for Modelling Electrosurgical Tissue Cutting

Author(s): Zhongqing Han, Venkata S. Arikatla, Suvranu De, *RPI*.

1. Introduction Electrosurgical tools are widely used in surgical procedures, in which radio frequency electric current is applied to divide tissue. A skilled surgeon should be able to perform surgery and limit inadvertent thermal damage and blood loss. However, current hands-on approaches to training electrosurgery are either expensive (in vivo) or lack of realistic fidelity (ex vivo). Computer simulation of electrosurgery promises low cost, safe and flexible training. However, previously proposed systems have limited physical fidelity, relying on geometric means of estimating tissue effects. Finite element modelling of electrosurgery procedures is capable of providing multiphysics based tissue effects, thus offering greater physical fidelity. A major challenge for finite element modelling of surgery is how topological changes are addressed during electrosurgical cutting. In this paper we present a local level set procedure as a potential solution. 2. Methods Our approach is based on finite element electro-thermo-elastic analysis of biological tissue. A co-rotational finite element model is used to simulate the elastic deformation of tissue. The electrical current and thermal-spread are similarly modeled using linear finite element models. Deformation and heat models can be decoupled because vaporization takes place much more quickly compared to the changes in tissue parameters due to thermal effects. However, the thermal and electrical models have similar time-scales and therefore must be coupled for accurate results. A localized level set method is used to track the divided tissue interface. The basic idea is to use the input electrical energy exerted by the electrosurgical tool as the evolving velocity field of the level set interface to control the width and depth of cutting tissue interface. 3. Results We have presented a multiphysics based finite element modelling of electrosurgery procedures, offering greater physical fidelity. A local level set procedure is used to track the cutting interface. References [1] F. Liane, F. Pascal, and J. Danie B., The SAGES Manual on the Fundamental Use of Surgical Energy (FUSE). Springer. [2] Z. Lu, V. S. Arikatla, Z. Han, B. F. Allen, S. De, A Physics-based Algorithm for Real-time Simulation of Electrosurgery Procedures in Minimally Invasive Surgery, Int. J Med Robot, 495-504, 2014. [3] S. Osher, J. Sethian, Level Set Methods and Dynamic Implicit Surfaces, Springer-Verlag, New York, NY, 2002.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Inflow Estimation for a 1D Arterial Network Model via Ensemble Kalman Filter

Author(s): Andrea Arnold, Christina Battista, Mette Olufsen, *North Carolina State U.*.

While many 1D fluid dynamics models have been implemented to predict blood flow propagation in arterial networks, it remains a challenge to determine proper parameters corresponding to physiological data. We investigate the impact of boundary conditions on such models by analyzing how network inflow can be predicted from measurements of blood pressure and area. More specifically, in a study where blood flow dynamics were not measured, we show how the inflow profile can be estimated given downstream measurements of pressure and area by viewing the problem from a Bayesian inverse problems perspective and applying a variation of the ensemble Kalman filter (EnKF). By employing an EnKF-based iterative scheme in the style of [1] in this setting, we are able to estimate the initial flow profile from a prior distribution of curves. The resulting posterior distribution of flow profiles yields an estimate for the mean flow profile using an ensemble of temporally discretized curves, along with a measure of the uncertainty in the estimation of blood pressure and area. The effectiveness of the proposed technique is demonstrated using blood pressure and area data obtained from the ascending aorta of a healthy male Merino sheep; for details of the experimental protocol, see [2]. References: [1] A. Arnold, D. Calvetti and E. Somersalo (2014) Parameter estimation for stiff deterministic dynamical systems via ensemble Kalman filter. Inverse Problems, 30 (10), 105008. [2] C. Battista, D. Bia, Y. Zocalo German, R. L. Armentano, M. A. Haider and M. S. Olufsen (2015) Wave propagation in a 1D fluid dynamics model using pressure-area measurements from ovine arteries. To appear in J Mech Med Biol.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Graphical System for Implementing Lumped Parameter Vascular Boundary Conditions: From Pen and Paper to the Supercomputer in Five Minutes

Author(s): Christopher J Arthurs, Rostislav Khlebnikov, *King's College London*; Kevin D Lau, *U. Michigan*; C Alberto Figueroa, *King's College London; U. Michigan*.

We report on the latest developments in user-friendly boundary condition specification within CRIMSON (CardiovasculaR Integrated Modelling and SimulatiON), an intuitive, powerful software environment which permits patient-specific simulation of haemodynamics. Specifying physiologically-accurate boundary conditions is a major area of research in cardiovascular modelling. A widely-used approach is to specify Lumped Parameter Network (LPN) models at boundaries, implemented via a coupled multidomain method [1]. Design considerations range from simple parameter tuning to ensure that mean flow and diastolic pressure decay are physiological, to more involved scenarios such as the design of elastance-based heart models, autoregulation of specific components, or lumped models of the venous system. While previous efforts have demonstrated how general LPN models can be applied [2], a major limitation has been that novel LPN designs must be converted into code by an expert developer. This approach is time-consuming, inaccessible, prone to error, and discouraging of exploration and curiosity. Addressing these issues, we have developed a GUI-based, drag-n-drop boundary condition specification system for CRIMSON, which allows the user to rapidly assemble LPNs from a toolbox of components containing resistances, compliances, inductances and valves, as well as to specify fixed pressure and flow waveforms. Complexity is hidden from the user; the LPN design is transparently and automatically translated into the equivalent boundary condition, with the system automatically determining whether Dirichlet or Neumann specification is appropriate. This development builds upon CRIMSON's existing user-friendly design, which allows even novice users to follow the patient-specific workflow from a vascular medical image stack, through individual vessel segmentation, meshing, and finally, to Navier-Stokes simulation. These new tools further enhance CRIMSON's capability for making haemodynamic simulation more accessible; for the first time, rapid prototyping and implementation of novel LPN boundary conditions can be performed quickly and robustly, by individuals who are not expert numerical analysts. [1] Vignon-Clementel, A coupled multidomain method for computational modeling of blood flow. PhD Thesis, Stanford University, (2006). [2] Moghadam et al. A modular numerical method for implicit 0D/3D coupling in cardiovascular finite element simulations. J Comp Phys, 244:63-79 (2013). We gratefully acknowledge support from the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement n. 307532, and the United Kingdom Department of Health via the National Institute for Health Research (NIHR) comprehensive Biomedical Research Centre award to Guy's and St Thomas' NHS Foundation Trust in partnership with King's College London and King's College Hospital NHS Foundation Trust.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Exact Representation of Interfaces Using Enriched Level-Set Technique

Author(s): Hossein Asadi Kalameh, *Cenaero/U. de Liège*; Olivier Pierard, *Cenaero*; Eric Béchet, *U. de Liège*.

This work aims to improve implicit representation of complex industrial work-pieces by reducing the existing gap between Computer Aided Design (CAD) and Computer Aided Engineering (CAE). The proposed approach is based on the level-set technique [1]. Limitations of the latter technique results in the miss-capturing of corners lying on the interface (iso-0 level-set) and other sharp features. These limitations also have a significant impact on surrounding elements. In order to avoid undesired over-smoothing to the sharp features, especially corners, an enhanced representation is proposed that is based on level sets method is introduced. This technique, referred in what follows by “level-set+” ,enriches the classical level-set by using data related to the corner points. This is done by automatically detecting geometrical points and using this information in the implicit representation. Elements containing these geometrical points and surrounding elements will be re-subdivided according to the updated iso-contour. This technique helps to employ classical level set and preserve current data structure for most of the creation of the iso-0 level set. Although the method is general enough to handle most possible configurations in terms of the corner locations, there are still limitations which have been handled in such a way to prevent computational failure. Also, the technique is effective at reducing the memory requirements by automatically erasing sharp features that are no longer existing after e.g. boolean operations. Some novel results illustrates accurate implicit representations of boundaries including the exact capture of sharp features in 2D and 3D. All the developments are implemented in our in-house finite element software Morfeo. There are numerous applications which can benefit from the above mentioned developments including crack propagation with the X-FEM method and transient machining simulations. [1] J.A. Sethian. Level set methods and fast marching methods: evolving interfaces in computational geometry, fluid mechanics, computer vision, and materials sci-ence.Vol. 3, Cambridge university press, 1999.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Multifunctional Optimization for Additive Manufacturing Through Combined Topology Optimization and System Design

Author(s): Ian Ashcroft, *U. Nottingham*.

In recent years Additive Manufacturing (AM) has provided a driver for Topology Optimization (TO) by providing a means of manufacturing the complex geometries that result from structural TO. The most common AM techniques currently used in industry are only capable of manufacturing from a single material, or in some cases from two materials of a similar type. However, one of the most active areas of research into AM processes currently, is the development of true multi-material AM. This would enable the manufacture of multi-functional components in a single process. This now raises the question of how to design for this new processing capability. This paper proposes an approach for the design of additively manufactured, multi-material parts with embedded functional systems (e.g., a structural part with structural health monitoring electronic/electrical components and associated conductive paths). One of the main issues to be addressed in the design of such parts is the coupling strategy that enables the structural TO to be coupled with the system design. This is achieved in the proposed method by accommodating the effects of system integration on the structural response of the part within TO. The coupled optimization strategy outlined in this work consists of: 1) a placement method used to determine suitable component locations (influenced by information extracted from the skeleton i.e. medial axis / surface of the structure), 2) a routing method for optimal shortest distance connections between points (here, a fast marching algorithm is used to route between two fixed points and an Ant Colony optimization is used to tackle the combinatorial problem with flexible component order), and 3) integration into a TO routine taking account of the effect of routing on structure and vice-versa. This paper will describe the progress in developing the proposed coupled optimization design approach and examples will be presented that will illustrate the benefits of the method, which include: optimal system design, miniaturization, circuit encapsulation (protection) and tailored structure-system performance.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Combined Deterministic and Stochastic Adaptation for Goal-Oriented Uncertainty Quantification

Author(s): Isaac Asher, Krzysztof Fidkowski, *U. Michigan*.

A new method for uncertainty quantification (UQ) that combines adaptivity in the physical (deterministic) space and the stochastic space is presented. The sampling-based method adaptively refines the physical discretizations of the simulations, along with adaptively building a stochastic model and adding samples. UQ studies can be very expensive due to complex physics requiring large physical solutions and due to a large number of parameters which results in a very large stochastic space to explore and model. The new UQ method can result in lower errors and lower cost by balancing different sources of error. By adaptively refining the physical and stochastic models, an overall prescribed error level can be reached without overly excessive and costly accuracy in either space. The UQ method takes advantage of an active linear subspace to reduce the dimensionality of the stochastic space while retaining relevant interaction terms and anisotropy. Driven by low-cost error estimates, a particle-swarm optimization method explores the stochastic space and drives adaptation that results in an efficient stochastic approximation. The UQ method is compared to to two modern methods for three test functions in a 100-dimensional space. The current method is shown to result in up to three orders of magnitude lower error and up to two orders of magnitude fewer samples. The UQ method is also used to assess modeling and discretization errors in a modified multiphase flow simulation. Based on an overall stochastic output of interest, the UQ method simultaneously drives adaptation of the stochastic and deterministic discretizations in order to balance the two sources of error. That is, terms are added to the stochastic model, samples are added, and the physical grid of each individual simulation is refined simultaneously. Error estimates based on semi-refined discretizations retain anisotropic accuracy, and a common grid is used to compare solutions from samples. The method for combined adaptivity performs well on the test problem, reducing the stochastic dimensionality from 20 to two and reducing deterministic errors on select samples. For about the same computational time, the method results in an order of magnitude less error and an order of magnitude fewer degrees of freedom compared to three other methods.

13th U.S. National Congress on Computational Mechanics
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Title: Non-Linear Stabilization of High-Order Flux Reconstruction Schemes via Fourier-Spectral Filtering

Author(s): Kartikey Asthana, Manuel Lopez-Morales, Antony Jameson, *Stanford U.*.

High-order Flux Reconstruction (FR) schemes have been limited in their application to transonic and supersonic problems on account of numerical instabilities related to the resolution of jump discontinuities. These instabilities arise from aliasing errors [1] associated with the collocation projection of the flux corresponding to the numerical solution onto the polynomial basis of the numerical flux. This presentation highlights the principal results from an ongoing investigation [2] which shows that these instabilities can be robustly suppressed using explicit physical filtering operations that preserve accuracy away from the discontinuities. Moreover, the computational effort is linear in the number of elements. We begin by obtaining energy bounds on the numerical solution via FR to prove that stability can be ensured for any polynomial order by the addition of adequate artificial dissipation such that the solution is energy-stable beyond a critical grid resolution. This artificial viscosity is then posed as a Fourier filtering operation which is implemented in the physical space via a strictly local convolution integral. A notable departure from previous filtering strategies is in the incorporation of edge information from neighboring elements in order to control inter-element discontinuities. The filter is selectively applied to ‘troubled’ cells as indicated by a discontinuity sensor based on the spectral concentration method [3]. Numerous numerical tests in 1-D and 2-D have been performed to validate the theoretical results. The proposed approach captures shock discontinuities while preserving accuracy in smooth regions of the solution, even for very high polynomial orders such as P=119. The filtered solution provides reduced total variation, reduced maximum overshoot/undershoot, and even allows sub-element shocks to be localized in the interior of an element. 1. A. Jameson, P. E. Vincent, P. Castonguay: On the Non-linear Stability of Flux Reconstruction Schemes. Journal of Scientific Computing, 50(2), 434-445 (2012) 2. K. Asthana, M. R. Lopez-Morales, A. Jameson: Non-linear stabilization of high-order Flux Reconstruction schemes via Fourier-spectral filtering. Under review at the Journal of Computational Physics 3. A. Gelb, E. Tadmor: Detection of Edges in Spectral Data. II-Nonlinear Enhancement. SIAM Journal of Numerical Analysis Vol. 38, No. 4, 1389-1408 (2000)

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Analysis of Material Defects in Micropolar Elastic Solids Using the Boundary Element Method

Author(s): Elena Atroshchenko, *U. Chile*; Jack S. Hale, Stéphane P. A. Bordas, *U. Luxembourg*.

The theory of micropolar elasticity is one of many generalized continuum theories, proposed by the Cosserat brothers [1] and later developed by Eringen [2] and others, that includes microrotations of material points as additional degrees of freedom and the couple-stress tensor to describe the deformation of an elastic solid. The constitutive equations contain intrinsic material length scale parameters, which characterize material microstructure and make the theory suitable for describing size-effects. In this work we develop a boundary element method framework for both, singular and hyper-singular boundary integral equations of plane micropolar elasticity and use it for analysis of stress concentration around voids, cracks and inclusions of a micropolar material. The equations of both types are used to model cracks with coincident crack faces. The equations on the boundaries of inclusions allow jumps in displacements and tractions, as well as the linear dependence of the boundary tractions on the boundary displacements, which is used to model various homogeneously imperfect interfaces. Numerical results for several benchmark problems, such as the problems of an infinite plate weakened by a single circular hole or a straight crack or a circular inclusion are shown to be in an excellent agreement with the known analytical solutions, while for more complex geometries the BEM-results are compared with the results obtained by the standard finite element method. REFERENCES [1] Cosserat E., Cosserat F. 1896. Sur la theorie de l'elasticite. Ann. de l'Ecole Normale de Toulouse, 10(1) [2] Eringen A.C. 1966. Linear theory of micropolar elasticity. J. Math. Mech. 15

13th U.S. National Congress on Computational Mechanics
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Title: Elastic Anisotropy and Low Symmetry Crystals in Dislocation Dynamics

Author(s): Sylvie Aubry, *LLNL*.

A multi scale modelling capability for predicting the strength of hexagonal close packed materials is being developed at Lawrence Livermore National Laboratory. This approach combines molecular dynamics and dislocation dynamics simulations with crystal plasticity to predict the strength of beryllium and magnesium for army applications. We will present an extension of the dislocation dynamics method to the treatment of hexagonal close packed (HCP) materials like Beryllium (Be) and Magnesium (Mg). All slip systems of the HCP structure are taken into account, a non-linear mobility law specific to Mg and Be is developed, and two topological operations are defined to treat HCP materials correctly. Large scale simulations will be presented and analysed for different straining conditions. These simulations are used in the construction of a constitutive law for a crystal plasticity model.

13th U.S. National Congress on Computational Mechanics
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Title: Boundary Layer Mesh Generation on Arbitrary Geometries

Author(s): Romain Aubry, Bilge Kaan Karamete, Eric L. Mestreau, Saikat Dey, *US Naval Rsch. Lab.*.

The work proposed in \cite{aubrycorner} is revisited. A new highlight is given to corner and ridge boundary mesh generation through the generalized Voronoi diagram in general and the spherical Voronoi diagram in particular. This provides the keystone to allow for the first time to generate boundary layers at arbitrary corner configurations. Numerical examples illustrate the accuracy and robustness of the method. This method seems to handle arbitrary geometry boundary layer generation, in theory as well as in practice.

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Title: Estimation of Fully Three-Dimensional Properties of Passive Myocardium: A Coupled Inverse Model-Experimental Study

Author(s): Reza Avazmohammadi, Samarth Raut, John Lesicko, Michael Sacks, *UT Austin*.

Knowledge of the three-dimensional (3-D) mechanical behavior of myocardium is essential to understand its physiology and pathophysiology, and to develop suitable biomaterials for replacement. Despite the significant progress made in the two-dimensional experimentation and modeling of myocardial tissues, substantial needs to obtain and model its full three-dimensional. A major challenge in this area is the complex architecture of the myocardium which endows myocardium with strongly anisotropic and heterogeneous properties. Currently, available experimental data for the mechanical properties of passive myocardium are planar biaxial and shear testing. While pivotal studies, there remains no current method to quantify the full 3D mechanical behavior of myocardium. Our aim in the present work is two-fold. First, based on a kinematical analysis, we obtain an optimal set of deformation modes, consisting of both shear and biaxial modes, and apply them to obtain new experimental data on the gross 3-D mechanical behavior of cubic samples of passive myocardium. Second, noting that these experiments produce noticeably inhomogeneous deformation fields inside the cubes, we develop an inverse finite element model based on an anisotropic Fung-type pseudoelastic energy function and accurately estimate the parameters involved. The energy function in our model is assumed to be locally orthotropic which is consistent with the (histologically-observed) myofiber-collagen fibers arrangement in the myocardium structure. A significant feature of our inverse model is that it is able to incorporate the histologically-measured spatial variation of local preferred material directions throughout the myocardium sample. In this connection, a series of finite element simulations are carried out to investigate how this variation influences the values of the estimated energy parameters in our model. We also conduct a comparative study of alternative sets of energy parameters to find an optimal set of parameters that are sufficient to capture the mechanical behavior observed in the experiment. Finally, we run additional experiments for some combined deformation modes and use the data to evaluate the descriptive capacity of our model.

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Title: Adaptive Wavelet Enhancement of the Classical Crystal Plasticity Finite Element Method Consistent with Error Patterns

Author(s): Yan Azdoud, Jiahao Cheng, Somnath Ghosh, *Johns Hopkins U.*.

Modeling complex polycrystalline microstructure requires a fine discretization to attain satisfactory accuracy. A global fine discretization increases dramatically the computational cost due to the large number of degrees of freedom and time steps. Efficient discretization is critical for problems that introduce localization, such as shear banding, twinning or fracture. We have developed an adaptive enrichment scheme that would selectively allocate degrees of freedom when and where necessary in the simulation. Fourier based methods have been recently introduced in crystal plasticity in order to accelerate the solving part of the simulation. However, such methods rely on a basis of global periodical functions that cannot capture local phenomenon with a high convergence rate. Hence, we adopted a local enrichment scheme. Wavelet decomposition is a suitable tool for data compression and analysis, and has been used successfully in meshless methods [1]. Second generation wavelets [3] resulted in significant progress with enhanced finite difference methods for highly non-linear fluid mechanics simulations [2]. We develop a new method based on second generation wavelets to enrich finite element simulations. In our method, a wavelet decomposition scheme is used to analyze error indicators in order to provide a basis of enrichment functions. The wavelet family is chosen such that the enrichment functions constitute a hierarchical finite element basis. These functions are introduced adaptively in the FEM scheme to locally enrich the solution. The novelty of this method is that the adaptive scheme is consistent with the error analysis. Our method is evaluated against a linear elastic benchmark problems and some numerical examples are given for crystal plastic behavior. [1] S. Li, S Ghosh, Extended Voronoi cell finite element model for multiple cohesive crack propagation in brittle materials, Int. J. Numer. Meth. Engng, 65, 7, 1028-1067, (2006) [2] O. Vasilyev, S. Paolucci, An adaptive multilevel wavelet collocation method for elliptic problems, Journal of Computational Physics, 206, 412-421, (2005) [3] W. Sweldens, The Lifting Scheme: A Construction of Second Generation Wavelets, SIAM J. Math. Anal., 29, 2, 511-546, (1998)

13th U.S. National Congress on Computational Mechanics
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Title: Modelling the Macro-Mechanical Axial Progressive Damage of Carbon/Glass Epoxy Circular Tubes

Author(s): Alia Ruzanna Aziz, Zhongwei Guan, Tawan Boonkong, *U. Liverpool*; Wesley James Cantwell, *Khalifa U. Sci., Tech. & Rsch.*.

The superior energy-absorption and crashworthiness properties of composite materials are of interest in a range of sectors, including those associated with the automotive and aerospace industries. There is a need for reliable finite element crushing models of composite materials in crashworthiness design as experimental testing is time consuming and rather costly. Current numerical codes for metallic materials are well understood and capable to predict the large plastic deformations and the crushing responses by applying elastic-plastic material models. However, the process of reproducing complicated composite failure mechanisms alongside with the friction effects causing the computational models of composite much more challenging than simulating conventional metallic materials. This work is focused on the modelling technique for complex composite structures of carbon/glass fibres epoxy circular tubes for use as lightweight reinforcement for foam sandwich structures. Axial progressive crushing analysis of five-ply composite tubes was simulated using commercial finite element package Abaqus/Explicit by employing Hashin damage criteria. The influence of several different parameters on the composite tubes modelling was analysed. The resulting load-displacement curves and the deformation responses of tubes were compared with previously published experimental crush results on carbon/glass epoxy tubes. Variation of the initial peak load and the sustaining crushing load were carefully examined. It is shown that the model adequately predicts the energy absorption of the composite tubes subjected to axial loading condition.

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Title: Phase-Field Models of Tumor Growth: The Effects of Biomechanical Stress Fields, Degradation, and Remodeling of the Macroenvironment

Author(s): Ernesto A B F Lima, J. Tinsley Oden, Danial Faghihi, *UT Austin*; Regina C Almeida, *LNCC* .

We have recently developed a ten-species tumor growth model using continuum mixture theory and phase-field approximations including models of angiogenesis [1]. In this presentation, we explore the influence of mechanical stress and deformation of the extracellular matrix (ECM) in tumor growth and compare growth and invasion patterns of solid tumors with and without models of mechanical deformation. These models depict the tumor environment as composed of different types of cells embedded in the ECM, linked by a variety of signal transductions. Cancer progression and invasion is a complex process involving an intricate interplay of a numerous signaling pathways, cell-cell and cell-microenvironment mechanical/chemical interactions. In order to grow, the tumor cells need to remodel their environment by interacting with the ECM and promoting the growth of new blood vessels as a new source of nutrients. We describe preliminary work in multiscale models, that establish the connections between cellular models and macroscale continuum models. The former takes the form of agent based models similar to those advocated by Macklin et al. [2]. We describe possible homogenization algorithms that allow the use of subcellular-level information to inform parameters of the tissue-level phase-field models. An issue of overreading importance is the numerical solutions of the often stiff and unstable system of equations generated by high-order models. We present stabilized algorithms designed to cope with these problems. The results of several numerical experiments are presented. [1] E. A. B. F. Lima, J. T. Oden and R. C. Almeida. A hybrid ten-species phase-field model of tumor growth. Math Models Methods Appl Sci, 24(13):2569 - 2599, 2014. [2] P. Macklin, M. E. Edgerton, A. M. Thompson, and V. Cristini. Patient-calibrated agent-based modelling of ductal carcinoma in situ (DCIS): From microscopic measurements to macroscopic predictions of clinical progression. J. Theor. Biol, 301(0):122 - 140, 2012.

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Title: Numerical Quantification of Hemodynamics and Wall Mechanics in Grafts of Coronary Artery Bypass Graft Surgery

Author(s): Abhay B. Ramachandra, Andrew Kahn, Alison Marsden, *UCSD*.

Coronary artery bypass graft surgery, a procedure performed on approximately 400,000 patients each year in the United States, revascularizes diseased coronary arteries using (in order of preference) arterial, venous or synthetic grafts. Many patients require multiple grafts and, due to the limited availability of arterial grafts, more than 70% of the procedures use vein grafts. However, approximately 40-50% of vein grafts fail in less than 10 years, and hemodynamics and wall mechanics are known to play a key role in this maladaptation. Hence, to non-invasively quantify clinically relevant hemodynamic quantities, such as wall shear stress and oscillatory shear index, we perform finite element simulations on patient-specific geometries derived from CT images. The 3D patient-specific domain is coupled to a 0D lumped parameter circulatory model [1] using an implicit modular 0D/3D coupling framework [2]. The lumped parameters are tuned to match patient-specific blood pressures, stroke volumes, heart rates from the clinic and heuristic flow-split values. We quantify differences in hemodynamics between arterial and venous grafts and discuss possible correlations to graft failure. Differences between a rigid wall simulation and deformable wall simulation will also be discussed. Quantifying hemodynamics and wall mechanics non-invasively is not only important for clinical diagnosis and treatment but is a necessary step towards coupling continuum models with cellular/subcellular models of growth and remodeling of blood vessels. [1] Sankaran, Sethuraman, Mahdi Esmaily Moghadam, Andrew M. Kahn, Elaine E. Tseng, Julius M. Guccione, and Alison L. Marsden. "Patient-specific multiscale modeling of blood flow for coronary artery bypass graft surgery." Annals of biomedical engineering 40, no. 10 (2012): 2228-2242. [2] Moghadam, Mahdi Esmaily, Irene E. Vignon-Clementel, Richard Figliola, Alison L. Marsden, and Modeling Of Congenital Hearts Alliance (mocha) Investigators. "A modular numerical method for implicit 0D/3D coupling in cardiovascular finite element simulations." Journal of Computational Physics 244 (2013): 63-79.

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Title: Discontinuous Galerkin Methods for Inverse Potential Problems

Author(s): Olalekan Babaniyi, Paul Barbone, *Boston U.*; Assad Oberai, *RPI*.

We consider the design of finite element methods (FEM) for inverse problems governed by elliptic forward operators with full-field data. For this class of problems, novel FEM methods have been proposed [1] and give good performance, provided the solutions are in the H1(Ω) function space, which does not allow for discontinuous or noisy distributions. The mechanical properties being estimated can be discontinuous in general. For this reason, it seems that a discontinuous Galerkin finite element (DGFE) approach, in which solutions are sought in more general function spaces that allow for discontinuities, has the potential to produce more accurate results. This presentation explores various stabilized DG formulations to solve this class of inverse problems. The stabilized methods considered include using upwinding [2, 3], more general least squares (LS) stabilizations, and a DG generalization of the adjoint weighted equation (AWE) formulation proposed in [1]. Numerical results and mathematical properties of the DG implementation of these methods will be compared to each other and to their continuous formulation counterparts. References [1] P.E. Barbone, A.A. Oberai, and I. Harari. Adjoint-weighted variational formulation for a direct computational solution of an inverse heat conduction problem. Inverse Problems, 23:2325–2342, 2007. [2] Franco Brezzi, Bernardo Cockburn, L Donatella Marini, and Endre S ■uli. Stabilization mechanisms in discontinuous galerkin finite element methods. Computer Methods in Applied Mechanics and Engineering, 195(25):3293–3310, 2006. [3] Franco Brezzi, L Donatella Marini, and E S ■uli. Discontinuous galerkin methods for first-order hyperbolic problems. Mathematical models and methods in applied sciences, 14(12):1893–1903, 2004.

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Title: Dynamic Cohesive Fracture Simulation for a Material with Microstructure by Using Mesh Adaptivity

Author(s): Hyunil Baek, Kyoungsoo Park, *Yonsei U.*.

Microstructure in a material provides significant impact on dynamic fracture behaviour because microstructure can change crack path, fracture toughness, etc. In order to consider microstructure of a material, multi-scale analysis approaches have been proposed because of the computational cost. However, most multi-scale methods suffer from boundary conditions between two length scales especially when localization like a crack is initiated. In this context, a multi-scale modeling approach is proposed by developing an adaptive mesh refinement technique. A microstructure of a material is adaptively inserted around crack tip regions through adaptive mesh refinements. Note that edges of a microstructure are accurately represented in conjunction with the Delaunay triangulation. While nodal connectivities of a finite element mesh are updated by using a topology-based data structure(TopS)[1]. The PPR potential-based cohesive zone model is employed for a traction-separation relationship across fracture surface[2]. Computational results demonstrates that microstructure of a material influences crack path and crack velocity.

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Title: Movement of Sheet Material in Rolling Pair

Author(s): Gayrat Bahadirov, *TSTU*.

Features of process deforming of resilience-plastic shafts under pressure between rotating rollers are not learned enough well. There are different approaches, which appear with researching of acquisitions, retraction and movement resilience-plastic shaft, comprising fluid components between rotating rollers. In calculations it was used general law of dynamics for shaft of variable-mass. The investigation of the process made, when a curve contact of deformation line between two rollers with identical radius represents as a parabola. Centre of gravity of sheet material, consequently, distinguished element always recumbent on the symmetry axis of sheet material. Therefore, equation of movement of distinguished element is enrolled in projection on this axis. The area of contact from geometry will be identified equalization of curved contact, in the form of parabola and acute angle of tilting about tangent. In general view defined the equation of tangent and normal line for parabola, passing through this point. By straight with defining equation tangent directed to the fictional force, and longitudinally straight normal reaction. The fictional force and reaction force will change its direction both in space and by time. Movement line of normal reaction does not pass through the center of the roller, under deformation of the rollers connecting in general. The normal line to parabola does not coincide with normal line to circumference, if movement lines of them pass through the same point with the exception of identified moment of time. Providing fictional force of sheet material about shaft and response of normal directed by normal line to parabola it is derived analytical solution of problem changing fluid mass in sheet material. On the basis of defined equation of movement of sheet material and variable-mass, it is found pressure of shafts on the element under consideration for arbitrary moment of time.

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Title: Evolution, Entrainment, Resuspension in Sediment-Laden Gravity Currents

Author(s): S Balachandar, Mrugesh Shringarpure, Nadim Zgheib, *U. Florida*; Mariano Cantero, Jorge Salinas, *Centro Atomico Bariloche*.

Sediment-laden gravity currents are driven by hydrostatic pressure differences between a sediment rich dense release and the surrounding clear fluid. Such flows are abundant in environment: turbidity currents, snow avalanches, dust storms and pyroclastic flows are some examples. For example, turbidity currents can be extremely energetic, erosive, carry large amounts of suspended sediments and propagate for long distances. As a consequence, they are considered to be one of the main mechanisms of sediment transport in the submarine environment. Consider the following description which elucidates the various complex mechanisms embodied in a turbidity current. As a turbidity current flows downstream it interacts with the ocean floor by entraining/detraining sediment by means of deposition (settling) and erosion (resuspension). At the same time the current is interacting with the surroundings by entraining ambient water at the top interface. Furthermore, within the current itself the suspended particles self-stratify and greatly modify turbulence. All these interactions are tightly coupled and are controlled by various factors like the amount of sediment load, properties of sediment, state of the ocean floor and ambient conditions. In our studies we have considered various large-scale numerical simulations that isolate these mechanisms for greater insights into their underlying role. We have analyzed the evolution of gravity currents when a finite volume of dense fluid is released in the ambient. We observe that the initial shape of the release and the topology of the floor to play a crucial role in the spreading/evolution of the current. These observations are compared against available experiments and shown to be consistent. The process of entrainment in sediment-laden currents can be quite different from other flows like jets and plumes. Numerical simulations of temporally growing turbidity currents in a tall channel have been performed to understand the role of Richardson number and settling velocity on the entrainment process. Finally, we also discuss modeling and simulation of resuspension flux for entrainment of sediment into the water column from the bed.

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Title: Morphoelastic Control of Gastro-Intestinal Organogenesis: Theoretical Predictions and Numerical Insights

Author(s): Valentina Balbi, Pasquale Ciarletta, *UPMC Paris* ; Ellen Kuhl, *Stanford U.*.

The intestine is one of the most structurally complex and fascinating organ in our body. His structural complexity is strictly related to the different functions it fulfills, as the nutritive and the absorptive, but also the immune. A variety of fascinating motifs pattern his inner surface since the early stages of embryo development. How those patterns arise and evolve remains poorly understood. In this work we propose an analytical model for the formation of different 1D and 2D patterns in the growing embryonic intestine. Our model is based on the hypothesis that these patterns arise as elastic instabilities induced in the tissue by the differential growth between its layers. Furthermore we show that not only mechanical but also geometric factors can explain intestinal pattern formation. Our approach is as follows. To allow for internal and external expansion, we model the embryonic gut as a two-layered hollow cylinder with stress-free boundaries: the inner layer represents the endoderm derived epithelium and the outer layer is constituted by mesoderm derived tissue and includes the mesenchyme and the muscle layers. Using the nonlinear field theories of mechanics, we model surface morphogenesis as the instability problem of constrained differential growth. To establish estimates for the folding pattern at the onset of folding, we perform a linear stability analysis supplemented by the perturbation theory. To predict pattern evolution in the post-buckling regime, we perform a series of nonlinear finite element simulations. Our model explains why longitudinal folds emerge in the esophagus with a thick and stiff outer layer, whereas circumferential folds emerge in the jejunum with a thinner and softer outer layer. In intermediate regions like the feline esophagus, longitudinal and circumferential folds emerge simultaneously. Our model could serve as a valuable tool to explain and predict alterations in esophageal morphology as a result of developmental disorders or certain digestive pathologies including food allergies.

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Title: Beam and Plate Modeling: An Approach Based on Dimension Reduction

Author(s): Giuseppe Balduzzi, Ferdinando Auricchio, Carlo Lovadina, *U. Pavia*.

Beam- and plate- modeling are classical problems of the continuum mechanics. Nevertheless, both standard and advanced models have several limitations, e.g., they provide too coarse description of the stresses, are not effective in accounting 3D or non-linear constitutive laws, and need correction factors. The presentation aims at illustrating a novel modeling procedure developed by Auricchio et al. [1, 2]. The main steps of the procedure are: 1. 3D linear-elastic problem formulation, among several possible weak problem formulations, the authors focus on the Hellingher Reissner functional dual formulation. 2. dimension reduction, a mathematical procedure that reduces the initial 3D problem to 1D or 2D problems, properly called beam- and plate- models respectively. 3. Finite Element discretization, standard 1D or 2D Finite Elements (for beams and plates respectively) are used to numerically calculate the model's solutions. Analytical and numerical results will highlight the main advantages of the dimension reduction procedure, summarized in the following. • An accurate description of stresses within the cross-section. • The possibility to take into account anisotropic 3D constitutive laws and to develop models effective also in general situations like non-homogeneous or non-prismatic beams and anisotropic plates [1, 2]. • The possibility to manage separately the model and the Finite-Element accuracies, consequence of the approximation of unknown-fields as the linear combination of cross-section- and axis- functions. • A clear and rigorous derivation path: the parameters required in modeling procedure are the domain's geometry and the material's mechanical properties. Unclear parameters and equation-terms or correction factors are unnecessary. • Robustness: a lot of numerical tests were performed demonstrating that the proposed model is effective in the most of cases of practical interest. • Accuracy in the description of displacements, stresses, and complex phenomena like stress concentration and local effects. • Superiority of the model’s numerical performances compared to classical 3D FE models. References [1] Auricchio, F., G. Balduzzi, M. J. Khoshgoftar, G. Rahimi, and E. Sacco (2014). Enhanced modeling approach for multilayer anisotropic plates based on dimension reduction method and Hellinger-Reissner principle. Composite Structures 118, 622–633. [2] Auricchio, F., G. Balduzzi, and C. Lovadina (2013). The dimensional reduction modelling approach for 3D beams: Differential equations and finite-element solutions based on Hellinger-Reissner principle. International Journal of Solids and Structures 50, 4184–4196. [3] Balduzzi, G. (2013). Beam Models: Variational Derivation, Analytical and Numerical Solutions. Ph. D. thesis, Univeristà di Pavia.

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Title: Modeling of Fiber Damage in Arterial Walls Based on a Relaxed Incremental Variational Formulation

Author(s): Daniel Balzani, Thomas Schmidt, *TU Dresden*.

Diseased arteries under supra-physiological loading, e.g. after a balloon angioplasty, show a macroscopic stress softening leading to permanent strains when unloading to the physiological state. This is believed to be the result of microscopic damage, mainly occurring in the embedded collagen fibers, when overstretching the artery. In order to incorporate this behavior into numerical calculations various models are proposed in the literature, which are mostly formulated in a classical continuum damage mechanics framework. Main drawback of such approaches is, that at certain deformations a loss of ellipticity and mesh-dependent solutions may be obtained. A way to solve this problem is the construction of relaxed incremental incremental variational formulations for damage, see e.g. [2], [3] for small strain approaches. In [1] an extension to large strains was derived for uni-directionally fiber-reinforced materials. Here, we extend this approach such that it is able to describe the softening behavior in arterial walls. For this purpose the model is modified to capture the stress-strain hysteresis observed in cyclic tests of arterial tissues. Then, dispersed fibers are considered and included in the formulation in terms of a microsphere-like model [3]. A flattened peanut-shape orientation distribution function is considered to account for different intensities of dispersion in tangential and radial direction of the arterial wall. In order to improve the numerical efficiency for the identification of the convexified incremental variational formulation an evolution strategy is combined with gradient-based minimization showing a significant improvement in robustness. Moreover, an approach for the efficient parameter adjustment is proposed and finally numerical examples will be presented to show the performance of the relaxed formulation. [1] D. Balzani, M. Ortiz. Relaxed incremental variational formulation for damage at large strains with application to fiber-reinforced materials and materials with truss-like microstructures. Int. J. Numer. Methods Eng. 92 (2012), 551-570. [2] G.A. Francfort, A. Garroni. A variational view of partial brittle damage evolution. Arch. Ration. Mech. Anal. 182 (2006), 125-152. [3] S. Göktepe, C. Miehe. A micro-macro approach to rubber-like materials. Part III: the micro-sphere model of anisotropic Mullins-type damage. J. Mech. Phys. Solids 53 (2005), 2259-2283. [4] E. Gürses, C. Miehe. On evolving deformation microstructures in non-convex partially damaged solids. J. Mech. Phys. Solids 59 (2011), 1268-1290.

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Title: An Analog of the Plane-Wave Method for Isolated Systems

Author(s): Amartya Banerjee, Ryan Elliott, Richard James, *U. Minnesota*.

In recent work, we have proposed a novel spectral scheme for solving the Kohn-Sham equations for isolated systems. This scheme, like the plane-wave method, is based on eigenfunction expansion and it allows accurate total energy calculations of clusters and molecules to be carried out systematically and efficiently without introducing any artificial approximations such as periodicity. We show in this follow up work how this scheme, like the plane-wave method, allows the definition of an energy cutoff parameter, with respect to which, monotonic convergence properties of ground state energies can be obtained. We also discuss computation of the Hellman-Feynman forces and it's convergence properties with respect to the energy cutoff in our method. Through examples, we demonstrate that specification of the energy cutoff in a standard plane-wave code and our code typically results in an agreement to < 1 micro-Hartree per atom in the ground state energies and < 0.5 milli-Hartree per Bohr in the Hellman-Feynman forces and that our code tends to perform more favorably in terms of execution time.

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Title: A Finite-Element Study of Deformation Behavior of Steel Specimens in Order to Obtain an Optimum Biaxial Tensile Test Specimen Design

Author(s): Dilip Banerjee, Mark Iadicola, Adam Creuziger, Timothy Foecke, *NIST*.

Lightweighting materials are increasingly being used by automotive companies as sheet metal components to meet fuel economy targets. However, verified material models are needed before these materials can be widely adopted. Verification of material models should be done under complex strain paths and plastic strains typically appropriate for traditional forming operations. Constitutive material model data are often developed with cross-shaped (cruciform) specimens. Optimum design of such specimens is a major goal of the present study. Finite element analysis (FEA) can serve as an effective tool for optimization of biaxial tensile test specimens. But FEA models need to be verified against experimental data. Calibrating FEA models against uniaxial tensile tests is a logical first step. Model predictions of strains and displacements in uniaxial specimens are compared with experimental data. In order to ascertain the effect of strain rates on deformation behavior, a dynamic, coupled temperature-displacement explicit finite element (FE) model of uniaxial specimens was developed. The Johnson-Cook flow stress model was used to model the constitutive behavior. Empirical parameters in the Johnson-Cook model are obtained from literature and adjusted through mathematical optimization. Role of imperfections in the FE model in developing the neck region is discussed. Next, FEA models of cruciform specimens are developed to simulate the deformation behavior in cruciform mechanical tests. Computed results of deformation, strain profile, and von Mises plastic strain agree reasonably well with measured values along critical paths in the specimens. FEA models correctly predict eventual failure locations in the cruciform specimens and provide insight into the plastic deformation behavior in the gauge area. Detailed analyses also suggest that the cruciform specimen thickness has an influence on the eventual mode of failure. A preliminary study summarizes recent progress toward shape or topological optimization of cruciform specimens by using calibrated and verified cruciform FEA models in conjunction with commercial optimization software

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Title: Isogeometric Inverse Formulation for Shell Structures

Author(s): Amir Barakati, *U. Iowa*.

Isogeometric Inverse Formulation for Shell Structures Amir Barakati and Jia Lu Department of Mechanical and Industrial Engineering The University of Iowa, Iowa City, IA, USA Abstract The inverse approach is an apt method for certain quasi-static mechanical and biomechanical problems. In the inverse method, the initial stress-free configuration and the stress in the deformed state are determined based on the known deformed configuration. Therefore, this approach is naturally suited to image-based, patient-specific applications such as human aneurysm stress analysis. In fact, the inverse method can be used as a stress solver for thin biomedical structures, in the sense that it enables the stress to be solved without knowing the realistic constitutive behavior of the material [1]. The isogeometric method has been proved to be a very powerful approach in computational mechanics. For shell structures the isogeometric method enables the development of displacement-only shell elements [2,3], which can be more efficient compared to traditional formulations with rotational degree of freedoms. Although the theoretical basis of an inverse nonlinear shell problem was previously developed, as far as isogeometric analysis is concerned, no work has been published related to the isogeometric inverse formulation of shell structures. In the present article, the NURBS-based mathematical framework for the inverse formulation of a finite strain Kirchhoff shell is presented. Since NURBS formulation is employed, the in-plain strain and curvature are directly computed from the displacement variables (i.e., control points). The strain energy is assumed to consist of separated contributions from the in-plane (membrane) and the out-of-plane (bending) deformations. The latter is defined based on the quadratic form of the surface curvature. The two components of the strain energy together with the virtual work of external loading are combined to formulate the weak form. The weak form is then linearized with respect to the deformed surface coordinates to yield the final FEM formulation. The developed formulation is demonstrated by several benchmark problems, followed by an example of aneurysm stress analysis. References [1] X. Zhou and J. Lu, “Inverse formulation for geometrically exact stress resultant shells” International Journal of Numerical Methods in Engineering, 74: 1278-1302, 2008. [2] J. Kiendl, K.-U. Bletzinger, J. Linhard, and R. Wüchner, “Isogeometric shell analysis with Kirchhoff-love elements” Computer Methods in Applied Mechanics and Engineering, 198:3902–3914, 2009. [3] D.J. Benson, Y. Bazilevs, M.C. Hsu, and T.J.R. Hughes, “Isogeometric shell analysis: the Reissner-Mindlin shell” Computer Methods in Applied Mechanics and Engineering, 199:276–289, 2010.

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Title: HPC System Design Using Analytics

Author(s): Wiliam Barth, James Browne, Todd Evans, Robert McLay, *UT Austin*; Robert DeLeon, Thomas Furlani, Steven Gallo, Amin Ghadersohi, Matthew Jones, Abani Patra, *U. Buffalo*.

Advanced computing centers around the world support a wide vari- ety of research projects in computational mechanics through the design, provisioning, and support of supercomputing systems. This talk discusses the evolution of a suite of tools and their application to the design of such systems and support of computational mechanics applications. This suite includes hardware and operating system data collected with a tool called TACC Stats, a job metadata tool called XALT, and data aggregation and presentation to users via a variety of web-based interface XDMoD. These tools together form the SUPReMM project. These tools have provided data to systems designers at TACC to classify and analyze the broad workload of applications on several systems, and this data has been used in the design of future TACC systems. This talk will describe the evolution of these tools and their applications to system design.

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Title: Combined Uncertainty and A-Posteriori Error Bound Estimates for General CFD Calculations

Author(s): Timothy Barth, *NASA Ames Rsch. Center*.

This presentation discusses the design and implementation of numerical methods for the quantification of statistical uncertainty, including a-posteriori error bounds, for output quantities computed using CFD methods. Hydrodynamic realizations often contain numerical error arising from finite-dimensional approximation (e.g. numerical methods using grids, basis functions, particles) and statistical uncertainty arising from incomplete information and/or statistical characterization of model parameters and random fields. The first task at hand is to derive error bounds for moment statistics given realizations containing finite-dimensional numerical error (Barth, 2013). The error in computed output statistics contains contributions from both realization error and the error resulting from the calculation of statistics integrals using a numerical method. A second task is to devise computable a-posteriori error bounds by numerically approximating all terms arising in the error bound estimates. A general software package for uncertainty quantification with quantified error bounds has been developed at NASA. The package provides implementations for a suite of numerical methods used in uncertainty quantification: * Dense tensorization basis methods (Tatang,1994) and a subscale recovery variant (Barth,2013) for piecewise smooth data, * Sparse tensorization methods (Smolyak,1963) utilizing node-nested hierarchies, * Multi-level sampling methods (Mishra,2010) for high-dimensional random variable spaces. The software provides the necessary tools and graphical user interface (GUI) for a user to rapidly pose uncertainty quantification problems to a CFD method and analyze the results of CFD computations. T.J. Barth,``Non-intrusive Uncertainty with Error Bounds for Conservation Laws Containing Discontinuities,'' \newblock Springer-Verlag Publishing, LNCSE, Vol 92, 2013. S. Smolyak,``Quadrature and Interpolation Formulas for Tensor Products of Centain Classes of Functions,'' Dok. Akad. Nauk SSSR, Vol. 4, 1963. M.A. Tatang,``Direct Incorporation of Uncertainty in Chemical and Environmental Engineering Systems,''' MIT, Dept. Chem. Engrg, 1994. S. Mishra and C. Schwab,``Sparse Tensor Multi-Level Monte Carlo Finite Volume Methods for Hyperbolic Conservation Laws,'', ETH Zurich, SAM Report 2010-24, 2010.

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Title: Image-Based Modeling of Skeletal Muscles Nased on Strong Form Reproducing Kernel Collocation Method for Hyperelasticity

Author(s): Ramya Rao Basava, J. S. Chen, *UC San Diego*.

In conventional meshfree methods based on the weak form, background meshes are required for the purpose of domain integration. Additionally, imposing essential boundary conditions requires special treatment since the meshfree approximation functions are usually not interpolating functions. This work introduces the meshfree strong form Reproducing Kernel Collocation Method (RKCM) for solving boundary value problems in context of nonlinear elasticity (hyperelasticity), for modeling human skeletal muscles using image data. The method is derived from minimization followed by linearization (using Newton's method) of the weighted least squares functional. In this work RKCM for nonlinear hyperelasticity is applied for modeling muscles of the human lower leg, in isometric contraction. The muscle models are constructed from segmentation of anatomical Magnetic Resonance (MR) images using level set based techniques. The pixel points obtained from these segmented MR images are used directly as nodes for domain discretization in the meshfree RKCM formulation. A hyperelastic constitutive law which incorporates the force stretch characteristics of skeletal muscles and allows for specifying the actual muscle fiber direction at each collocation point is used. In this work the muscle fiber directions are obtained from Diffusion Tensor Imaging data and are input directly at each pixel (collocation) point, without the need for further interpolation or processing.

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Title: Strain Localization in the Presence of Microstructural Evolution

Author(s): John Bassani, *U. Pennsylvania*.

A model is developed for a class of anisotropic elastic-plastic solids in which the orthotropic triad that characterizes the symmetry of the microstructure evolves with deformation. Microstructural spin is taken to be the difference between the material spin and plastic spin. A key relationship between plastic rate of stretching and plastic spin is derived utilizing representation theory for tensor-valued functions. As a consequence, microstructural evolution arises from non-coaxiality between the plastic rate of stretching and the orthotropic axes, which makes sense. The resulting phenomenological theory extends classical theories of anisotropic plasticity to include the evolution of the orthotropic axes. For loading in the plane of a textured polycrystalline sheet or for axial loading of a thin tube, only 2 additional material parameters are required for stressing in one of orthotropic symmetry planes,. Comparisons with experimental data are excellent. Predictions for necking, shear banding, and buckling display significant effects of microstructural evolution on strain localization. Important applications arise in automotive “light-weighting,” and detailed simulations that include microstructural evolution in tube crushing show promise in developing new design concepts. If time permits, recent work on microstructure evolution in complex fluids also will be discussed.

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Title: Extracting Various Similarity Formulations from an Extensive Database of Direct and Large-Eddy Simulations of Stably Stratified Flows

Author(s): Sukanta Basu, Ping He, *North Carolina State U.*.

Similarity theory is one of the cornerstones of boundary layer meteorology. Over the years, a variety of similarity formulations have been proposed in the literature, including (but not limited to): Monin-Obukhov (M-O) similarity theory, local scaling hypothesis, mixed layer scaling, and spectral scaling. All these formulations not only play critical roles in advancing fundamental turbulence research, they also have immense impact on a wide range of engineering and industrial applications. For example, the M-O similarity formulation of the refractive index structure parameter (Cn2) is widely used in the laser beam propagation field. The same formulation is also utilized for the (indirect) estimation of evapotranspiration, and thus, contributes to water resources management. Most of the existing similarity formulations have been empirically derived based on observational data collected during different field campaigns. It is needless to point out that these types of data are always susceptible to instrument noise, representativeness error, mesoscale disturbances, and other undesirable effects. In addition, ad-hoc assumptions (e.g., Taylor's hypothesis) are often required when one deals with observational data. Thus, it is not surprising that there is no general consensus in the contemporary literature regarding the exact shape/form of most of these similarity formulations. In principle, one could circumvent the aforementioned challenges by deriving the similarity functions from a numerically-generated database of high-resolution turbulent flow fields. We have created such a database using a newly developed direct numerical simulation (DNS) solver and a well-established dynamic (tuning-free) large-eddy simulation (LES) code. Our database contains more than one hundred and twenty simulations spanning a wide range of stabilities (from near-neutral to very stable). Both continuously turbulent and (globally) intermittently turbulent cases are represented in this extensive database. Several similarity formulations (ranging from gradient-based local scaling hypothesis to boundary layer height formulation) have been derived from this database. Interestingly, despite the fundamental differences between the DNS and LES methodologies, most of the extracted similarity formulations from these numerical approaches are found to be remarkably similar. Furthermore, they are also (qualitatively) comparable to the traditional observational data-based ones. The pros and cons of the proposed DNS/LES-based similarity formulations will be the focus of our presentation. In addition, we will also comment on the effects of Reynolds number and global-scale intermittency on the proposed similarity formulations.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Optimal Design of Polymeric Laminates for Maximum Energy Dissipation Under Low-Velocity Impact

Author(s): Romesh Batra, Guillaume Antoine, *Virginia Tech*.

A challenging problem in designing transparent laminates is to find the layup of polycarbonate (PC), polymethylmethacrylate (PMMA) and adhesive layers to maximize specific energy dissipation for low velocity impact. The problem is compounded by the fact that energy dissipation due to viscous deformations of the adhesive, plastic deformations of the PC and cracking in the PMMA are quite different, and they vary with time elapsed from the instant of impact. The adhesive layer allows only a part of the incident wave to be transmitted through it because its acoustic impedance is much lower than that of the PC and the PMMA. The optimization problem requires verified and robust computational algorithms and validated mathematical models for ascertaining time history of the energy dissipation. We have developed a mathematical model for analyzing the impact response of PC/adhesive/PMMA laminates and implemented it in the LS-DYNA (Low Speed Impact of Laminated Polymethylmethacrylate/Adhesive/Polycarbonate Plates, Composite Structures, 116, 193-210, 2014). The PMMA and the PC are modeled as elasto-thermo-visco-plastic and adhesives as viscoelastic. Failed elements are deleted from the analysis domain. Values of material parameters of the PMMA and the PC are taken from the literature, and those of adhesives determined from their test data (Constitutive Relations and Parameter Estimation for Finite Deformations of Viscoelastic Adhesives, J. Appl. Mechs., 82, Art. 021001, 2015). Delamination at interfaces is simulated by using a bilinear traction separation law. The model has been validated by comparing computed deformed shapes of the transparent laminates with experimental results. However, the sensitivity analysis has indicated that material parameters that strongly influence laminate's deflections are different from those that determine the energy dissipated (Sensitivity Analysis of Low-velocity Impact Response of Laminated Plates, Int. J. Impact Engng., 78, 64-80, 2015). The principal source of energy dissipation is found to be plastic deformations of the PC. The energy dissipated due to cracking of the PMMA is much lower than that due to plastic deformations of the PC. The energy dissipation in the adhesive is essentially negligible as compared to that in the PC and the PMMA. The optimization problem has been simplified by assuming that every layer has the same thickness. Here we use the genetic algorithm to find their layup for maximizing the energy dissipation under the constraint of fixed number of layers (Composite Structures, 124, 29-34, 2015). It is found that the configuration with the PC layer facing the impactor optimizes the energy dissipated.

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Title: Multi-Scale Treatment of the Effects of Temperature and Strain-Rate on the Plasticity of BCC Refractory Metals

Author(s): Corbett C. Battaile, Hojun Lim, *Sandia Nat'l. Lab.*; Christopher Weinberger, *Drexel U.*.

Metals that form the body-centered cubic (BCC) crystal structure usually exhibit strengths (e.g. yield stresses) that depend strongly on temperature and strain rate. This is due primarily to the "lattice friction," i.e. activation barrier, that must be overcome to move screw dislocations inside the material, and thus produce plastic deformation. Screw dislocation motion in these materials occurs by the formation and propagation of kinks along the dislocation line, and the (relatively) large activation barrier arises from the spatial dissociation of the screw dislocation cores. In this paper, we present a multiscale model for describing the temperature and strain-rate dependence of the yield strength of the BCC refractory metals molybdenum, niobium, tantalum, and tungsten. The model is based on physical concepts associated with dislocation-scale plasticity, specifically in regard to the dependence of dislocation kink pair formation on temperature and strain rate. We will describe the model formulation, its implementation in crystal plasticity finite element analysis, the calibration of continuum strength models (Johnson-Cook, Zerilli-Armstrong, and Mechanical Threshold Stress) to the crystal plasticity results, and predictions from ALEGRA [1] continuum solid dynamics simulations of Taylor cylinder impact that can be compared directly to available experimental measurements [2]. This represents a multiscale treatment of BCC plasticity that is based on concepts at the dislocation scale and ultimately provides calibration data for strength models in validated continuum simulations. [1] <http://www.cs.sandia.gov/ALEGRA/Alegra_Home.html> [2] P.J. Maudlin, J.F. Bingert, J.W. House, and S.R. Chen, "On the modeling of the Taylor cylinder impact test for orthotropic textured materials: experiments and simulations," Int. J. Plast. 15 (1999) 139-166.

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Title: Accounting for Energy Losses Associated with Wall Viscoelasticity by Estimating Boundary Conditions in One-Dimensional Arterial Networks

Author(s): Christina Battista, Mansoor Haider, Mette Olufsen, *North Carolina State U.*.

The ability to predict arterial blood pressure and flow pulse wave propagation in conjunction with wall mechanics via means of patient-specific modeling can enhance our understanding of cardiovascular diseases and potentially impact diagnostic techniques. To produce clinically useful estimates, the mathematical models must be complex enough to accurately describe the major network geometry along with elastic and viscoelastic wall properties in each vessel yet simple enough to allow for rapid computation. In this study, this balance was achieved by formulating a 1D fluid dynamics model coupled with elastic and viscoelastic wall models [1]. Typical 1D models are hyperbolic, requiring boundary conditions at the inlet and outlet of each vessel. At the proximal end of the vessel, a periodic flow profile is applied while a three-element Windkessel, comprised of two resistors and a capacitor, is prescribed at the distal end. It is well known that the model is sensitive to these boundary conditions as well as the parameters associated with the wall model. Biomechanical properties of the wall change along the axial direction, making vessels stiffer and less viscoelastic as you propagate throughout the network. When changing mechanical properties in the arterial wall, in particular viscoelasticity, various amounts of energy are lost throughout the system. This energy loss must be compensated for in the downstream vasculature via means of the outflow boundary conditions. To investigate how the viscoelastic wall impacts the outflow boundary conditions, the amount of viscosity is decreased until an elastic wall model is achieved while maintaining the same Windkessel parameters. Next, we match pulse pressure by adjusting the proximal resistor and mean pressure by varying the distal resistor. This study shows how variation of outflow conditions as well as wall model properties affect blood pressure and flow wave propagation. Specifically, we show how flow and pressure change under elastic versus viscoelastic wall models and how predictions of flow and pressure depend heavily on outflow boundary conditions. [1] C. Battista, et al. Wave Propagation in a 1D Fluid Dynamics Model Using Pressure-Area Measurements from Ovine Arteries. J Mech Med Biol 15(5): 1650007, 2014.

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Title: Enabling Large-Scale Complex Predictions Using Open-Source Software Elements

Author(s): Paul Bauman, *U. Buffalo, SUNY*; Roy Stogner, *UT Austin*.

In this talk, we describe efforts and challenges to bring together open-source software elements and develop extensible frameworks for enabling scalable multiphysics finite element simulations for making predictions of complex phenomena. Such predictions require not only enabling scalable algorithmic and software elements for the forward problem, but also infrastructure for enabling parameter variation and computations of gradients of quantities of interest. These capabilities allow enhanced sampling to assess parameter sensitivity, development of probability distributions of material coefficients (inverse analysis), and uncertainty assessments on quantities of interest (forward UQ). We focus on the open-source multiphysics package GRINS that is built on the libMesh finite element library, heavily uses PETSc, and interfaces QUESO all together to enable complex prediction capabilities. In particular, we describe efforts in enabling unstructured geometric multigrid using adaptive meshes generated by libMesh in concert with PETSc's composable solver framework. We describe impact of the integration with modular libMesh facilities for computing discrete adjoints and how these facilitate QoI-based error estimation and adaptivity as well as gradient enhanced sampling in solving Bayesian inverse problems. We illustrate these advances through several examples.

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Title: Modeling of the Transient Energy Release Due to Damage Initiation

Author(s): Jefferson Cuadra, Konstantinos Baxevanakis, Dani Liu, Antonios Kontsos, *Drexel U.*.

The sudden release of energy due to crack initiation and the associated transient stress wave propagation is known as Acoustic Emission (AE), which is a widely used nondestructive method. Similar to crack initiation, other dynamic deformation and damage mechanisms including dislocation motion, phase transformations, twinning, delamination and many others have been associated with experimental recordings of AE activity captured (passively) by the use of several sensors including piezoelectric, MEMS devices and fiber bragg sensors. Although such recordings of energy release related to AE are relatively straightforward, the inverse problem of finding the actual source is challenging due to both the sensing process itself (hardware and software influence) as well as due to the influence of geometry, material nonlinearities, inhomogeneities and anisotropy. To this aim, computational models that could assist in the characterization of the information carried by AE are of importance to understand the dynamic process of (micro)structure evolution and progressive failure due to the application of external loading. In this context, this talk presents cohesive-based 3D finite element models for both crack initiation in a fracture toughness setting and delamination in a structural component for the investigation of AE-related wave propagation due to damage initiation. The first model presented simulates a Mode I ductile fracture on a compact tension geometry using a 3D cohesive zone and a cohesive-based extended finite element approach, while it relies on a traction separation law constructed from full field strain and displacements obtained experimentally by digital image correlation. The second model consists of an aerospace skin stiffener panel to simulate delamination at the bond-line using a tuned traction separation law from the adhesive material properties. The computational AE source modeling methodology consists of defining damage initiation states from static simulations and linking such states to dynamic formulations in order to evaluate the wave propagation due to nucleation of the failure mechanism. Both type of models provided primitive AE signals which were analyzed in time, frequency and joint time-frequency domains. The simulated “forward problem” type AE signals are further compared to experimental AE waveforms by taking into account the signal conditioning created by the use of piezoelectric sensors; results are evaluated in the context of the "inverse problem" of source identification given recorded nondestructive data providing critical information about specific fracture mechanism.

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Title: Probabilistic Descriptions of Meso-Scale Material Properties Fields Using the Principle of Maximum Entropy

Author(s): Sarah Baxter, Katherine Acton, *U. St. Thomas*.

Accurately describing the macroscale structural behavior and variability resulting from random microstructure in heterogeneous composites is a significant research challenge. Mesoscale continuum material modeling can provide a basis for simulation of random material property fields, which can be used as input into an uncertainty analysis. One mechanism for developing a random field of properties is to homogenize at the level of statistical volume elements (SVE). A set of statistical volume elements (SVE) can be created by partitioning a representative volume element (RVE) into subvolumes. A hierarchy of bounds can be stated such that as the SVE length scale increases, the ensemble average of the effective properties of these volumes under kinematically uniform and statically uniform boundary conditions form upper and lower bounds, respectively, on the effective properties of the RVE . To make use of this approach requires the selection of a partitioning scheme that defines the mesoscale elements; partitioning options include different length scales and geometries. Using the principle of maximum entropy (PME), probability density functions (PDF), which characterize the distribution of effective properties in the collection of SVEs under different partitioning schemes, are developed. This work examines the effect of variation in partitioning length scale and geometry on the PDF of the mesoscale material property parameters.

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Title: Fluid-Structure Interaction of Wind Turbines: Recent Results and New Directions

Author(s): Yuri Bazilevs, *UC San Diego*.

Wind turbines convert the energy contained in the wind stream to electric power. These machines are designed for small-scale (kW range) and large-scale (MW range) power production, with rotor radii ranging from a few meters to a hundred meters in current offshore designs. There are many engineering challenges associated with the mechanics of wind turbines, both on the structural as well as aerodynamics sides. This presentation will focus on our recent efforts to address some of these challenges through advanced fluid-structure interaction (FSI) simulation. The core computational technology we developed, which includes isogeometric analysis (IGA) and moving-domain FSI, and is relevant to wind-turbine modeling, will be briefly reviewed. Recent computational results showing the power of the modeling techniques will be presented. The presentation will conclude with our recent efforts to go beyond the core techniques developed for wind-turbine FSI to include atmospheric boundary layers, coupling with ocean waves, and damage prediction in wind-turbine blades made of composite materials.

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Title: Unsteady Residual Distribution Schemes Adapted to Immersed Boundary Methods on Unstructured Grids to Account for Moving Bodies

Author(s): Héloïse Beaugendre, Léo Nouveau, Cécile Dobrzynski, Mario Ricchiuto, *Inria Cardamom*; Rémi Abgrall, *U. Zürich*.

The interest on immersed boundary methods (IBM) increases in Computational Fluid Dynamics because they simplify the mesh generation problem when dealing with the Navier-Stokes equations. To give a few examples, they simplify the simulation of multi-physics flows, the coupling of fluid-solid interactions in situation of large motions or deformations. Nevertheless an accurate treatment of the wall boundary conditions remains an issue of the method. In this work, a penalty term added to the Navier-Stokes equations accounts for the wall boundary conditions and accuracy is recovered using unstructured mesh adaptation. When a penalization technique is used as an IBM, the idea is to extend the velocity field inside the solid body (penalty term) in order to enforce rigid motion of this body. A level set function, the sign distance function to the solids, is used to capture interfaces of the solid bodies. Our numerical simulations are performed on unstructured anisotropic meshes (2D-triangles or 3D-tetrahedra) and we propose to combine our level-set based penalization approach to mesh adaptation [1]. The idea is to conserve the simplicity of the embedded approaches for grid generation process and overcome the difficulty of wall treatments by using mesh adaptation. Mesh adaptations are performed using two criteria, the distance to the level-set 0 (interface of the solid body) and the quality of the flow solution (Hessian of the velocity component or the density). Using some test cases we demonstrate the ability of the proposed method to obtain an accurate solution along with an accurate wall treatment even when the initial mesh does not contain any point on the level-set 0. Residual distribution schemes on unstructured meshes [2] are used to solve the equations: an implicit scheme for steady flows and an explicit one along with a specific splitting algorithm for penalized unsteady flows. Those numerical schemes allow the construction of a high order method with compact stencil to ease parallelism. Validations of the proposed method are performed using static and moving bodies. [1] R. Abgrall, H. Beaugendre, and C. Dobrzynski. An immersed boundary method using unstructured anisotropic mesh adaptation combined with level-sets and penalization techniques. JCP, 257:83–101, 2014. [2] M. Ricchiuto and R. Abgrall. Explicit Runge-Kutta residual distribution schemes for time dependent problems: second order case. JCP, 229(16):5653–5691, 2010.

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Title: Modeling Genesis of Natural Fractures Using XFEM

Author(s): Hao Huang, Varun Gupta, Rodrick Myers, Gauthier Becker, *ExxonMobil* .

Natural fractures can significantly impact a reservoir's productivity by either creating high permeability conduits, or conversely forming flow barriers due to cementation. Good understanding of natural fracture distribution, orientation, connectivity, and conductivity allows operators to reduce risk in exploration settings, improve completion planning, and drill more productive wells. A forward model which can simulate an arbitrary number of fracture initiations, interactions, and intersections plays a key role in predicting salient characteristics of a subsurface natural fracture network. In this talk, we will present several numerical techniques which allow us to simulate genesis of natural fractures during the geological process of burial and exhumation. Specifically, we will discuss the XFEM formulation to model fracture interaction and the tracking of fracture growth in 3D. The validity of the proposed method will be demonstrated by comparing fracture prediction with experimental and analytical results (e.g. shear lag model). The proposed model allows us to explore and quantify factors that control the density and connectivity of natural fractures. For example, in a multilayer setting we found that interlayer friction may severely suppress fracture interaction. Hence, a fracture simulation which does not consider the friction between layers (such as in most two dimensional fracture interaction studies) may exaggerate fracture connectivity and mislead the geological interpretation of fracture network connectivity in the subsurface.

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Title: Investigation of Yield Surface Characterization for Dynamic Strain Localization

Author(s): Richard Becker, *US Army Rsch. Lab.*.

The role of yield surface characterization in predicting strain localization in dynamic loading is investigated through the use of models with modified yield surface curvature and yield surface vertex effects in a several application-oriented loading configurations. The models represent a variety of previously established approaches intended to facilitate localization, focusing on the tensor aspects of the constitutive representation. Inertial effects at extreme loading rates can impede or expedite a shift to a localized deformation mode, depending on the geometry and loading. The dynamics continue to play a role in the post-localization response. Material properties which affect localization at low rates, such as strain rate sensitivity and strain hardening, are also investigated in the dynamic loading regime.

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Title: Effect of Annealing on Mechanical Properties of Polygraphene

Author(s): Matthew Becton, Xianqiao Wang, *U. Georgia*.

As the grain boundaries in graphene-related 2D materials can strongly affect their material properties and the performance of graphene-based devices, it is highly desirable to better understand the effects of grain boundaries and endeavor to make them as stable as possible. We discuss the application of molecular dynamics simulation to explore the annealing process of polygraphene and compare the mechanical properties of annealed and unannealed polygraphene to those of pristine graphene under the same conditions. We focus on the stability and energy of the grain boundaries over the course of the annealing process. Polygraphene with average grain sizes of 2, 3, 4, 6, 8, and 12 nm are annealed and run through a tensile test, with careful attention to the changes along the grain boundaries. Our results show that the annealing process has a strong effect on the strength and stiffness of polygraphene due to the rearrangement and stabilization of the grain boundaries. Irrespective of grain size, the annealing process makes polygraphene both tougher and stiffer, with a higher Young's modulus, strength, and ultimate strain under a tensile test compared to the same samples prior to the annealing process. We demonstrate that annealing is not only an important process to make the most stable structures experimentally, but also to make the most realistic structures computationally. With our work we hope to encourage rapid, low-cost annealing processes in order to find the most beneficial manner in which to utilize polycrystalline graphene, the preparation of which is more cost- and time-efficient than that of pristine graphene.

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Title: Quasicontinuum Methods for Planar Beam Lattices

Author(s): Lars Beex, Stéphane Bordas, *U. Luxembourg*; Pierre Kerfriden, Claire Heaney, *Cardiff U.*.

The quasicontinuum (QC) method is multiscale approach for lattice models that fully resolves lattice models in regions with individual lattice events and coarse-grains elsewhere. The QC method was originally proposed to reduce the computational costs of atomistics and has so far mainly been used for this. Recently however, the QC method has been reformulated in terms of virtual-power to deal with dissipation mechanisms. In this way the QC approach can also be used for structural lattice models using dissipative springs, e.g. for electronic textile and paper materials. A significant amount of structural lattice models use beams, in contrast to springs, depending on the material one desires to model. Whereas the kinematic variables of spring lattices are only formed by nodal displacements, those of beam lattices consist of nodal displacements and nodal rotations. Consequently, QC approaches for beams need to deal with the nodal rotations as well. Furthermore, when planar beam lattices experience out-of-plane deformation, the nodal displacements and nodal rotations are nonlinear functions of the nodal coordinates. This means that QC approaches for beam lattices require higher-order interpolation. Consequently, standard summation rules do not suffice. This presentation will show a number of QC formulations to deal with the typical issues arising in planar beam lattices and clearly distinguishes between the error due to interpolation and the error due to summation. Finally, the QC formulation most convenient in terms of accuracy versus efficiency, is presented.

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Title: Hemolysis Modeling in the Context of Benchmark Rotary Pumps

Author(s): Marek Behr, Lutz Pauli, Stefan Haßler, *RWTH Aachen U.*.

Modeling and computational analysis play an increasingly-important role in bioengineering, particularly in the design of implantable ventricular assist devices (VAD) and other blood-handling devices. Numerical simulation of blood flow and associated physiological phenomena has the potential to shorten the design cycle and give the designers important insights into causes of blood damage and suboptimal performance. A set of modeling techniques is presented which are based on stabilized space-time finite element formulation of the Navier-Stokes equations. Alternate methods that represent the rotating components in an averaged sense using a rotating frame of reference will be discussed. In order to obtain quantitative hemolysis prediction, cumulative tensor-based measures of strain experienced by individual blood cells must be developed; red blood cells under shear can be modeled as deforming droplets, and their deformation tracked along pathlines of the computed flow field. An efficient continuum-based approach is presented as an alternative to previous pathline-based methods. The methods are applied to simplified rotary blood pumps, one of which is currently a subject of an FDA round-robin study.

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Title: A Survey of Errors in Finite-Element Computations of Wave Propagation

Author(s): Stephen Beissel, *Southwest Rsch. Inst.*.

In addition to dispersion and dissipation, computations of wave propagation suffer from spurious oscillations commonly referred to as the Gibbs phenomenon. As wave fronts become more abrupt, like shocks, the spurious oscillations intensify. It has long been known that these oscillations are due to inadequate resolution of the wave fronts by the discretizations inherent to all numerical approximations. Since computing power is limited, it is generally not possible to avoid the oscillations by simply increasing mesh refinement. Instead, various forms of damping and filtering are typically used. These methods, however, are not able to distinguish between real and spurious oscillations, and they reduce or remove both kinds equally. In an effort to better understand the sources of errors in computations of wave propagation, this study surveys the growth of errors due to various algorithms and numerical parameters. Problems with analytic solutions are chosen, so that errors can be quantified by a suitable error norm. The emphasis is on waves resulting from impacts, since they hold great practical significance, and they suffer most acutely from spurious oscillations. The analyses in this study are performed on existing algorithms, but the objective is to guide the development of algorithms that accurately represent real oscillations, while avoiding spurious ones. Elements with higher-order shape functions have been shown to provide superior accuracy for some problems. In this study, the accuracy advantage of higher-order elements is shown to diminish as wave fronts become increasingly abrupt, resulting in reduced accuracy with increasing element order for computations of shock propagation. Errors are also analyzed for several explicit time-integration schemes, with differing orders of accuracy, for both consistent and diagonalized (lumped) mass matrices, and for both continuous- and discontinuous-Galerkin element formulations. Parametric variations include refinement of the mesh (accompanied by refinement of the timestep for a constant CFL number), and well as independent refinement of the timestep. Among the findings, it is shown that the errors due to the time-integration scheme do not always compound those due to the spatial discretization; they sometimes offset each other. Plots of the error norm as a function of timestep size demonstrate this synergy when the error norm decreases from its asymptotic value at small timesteps as the timestep is increased to the limit of stability. Other findings include a strong advantage to one form of the mass matrix, depending on the time-integration scheme.

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Title: On Mixed Isogeometric Analysis of Poroelasticity

Author(s): Yared Bekele, Trond Kvamsdal, Steinar Nordal, *Norwegian U. Sci. & Tech.*; Eivind Fonn, Arne Morten Kvarving, *SINTEF ICT*.

Isogeometric finite element analysis of poroelasticity was first presented by Izral et al. 2013. The advantages gained, due to the smoothness the basis functions, over the standard finite element method were highlighted, all while using equal orders of interpolation for the displacements and pore pressure. In the finite element method, using different orders of interpolation helps in achieving stability but the use of lower order pressure interpolation leads to a lower solution accuracy. In this contribution, we present a mixed isogeomteric formulation for poroelasticity problems and explore the use of different orders of interpolation for the field variables, with a view to assessing the accuracy of the results for very small time steps. Numerical studies are performed on one and two-dimensional consolidation problems.

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Title: Enabling Complex Applications on Heterogeneous Clusters with OmpSs MPI Offloading

Author(s): Vicenç Beltran, Jesus Labarta, *BSC*.

Exascale performance requires a level of energy efficiency only achievable with specialized hardware. Hence, to build a general-purpose HPC system with Exascale performance it will be necessary different types of processors, memory technologies and interconnection networks. Heterogeneous compute nodes are already present on some top supercomputer systems that usually combine multi-core processors and hardware accelerators such as GPUs or Xeon Phis. The DEEP Exascale project [1] has pushed this trend further by proposing heterogeneous cluster architectures to achieve Exascale performance. However, most HPC applications use MPI to implement a rigid Single Program Multiple Data (SPMD) execution model that does not properly fit on a heterogeneous cluster. Although, MPI-2 provides a powerful and flexible MPI_Comm_spawn() API that was designed to dynamically exploit heterogeneous clusters, its high complexity has hindered a wider adoption of this API. Hence, heterogeneous clusters are much harder to program and exploit than homogeneous ones, mainly due to lack of proper tools to map different parts of an application to different types of compute nodes. The DEEP Exascale project has tackled this problem extending OmpSs with convenient offloading features that are built on top of MPI_Comm_spawn(), thus easing the incremental port of existing MPI applications to heterogeneous clusters. The OmpSs programming model [2] can be used to dynamically offload MPI kernels, replacing low-level and error prone MPI_Comm_spawn() calls with high-level and easy to use OmpSs pragmas. Our extensions dramatically simplify the dynamic offloading of MPI kernels, showing competitive performance and scaling to a high number of nodes. The presentation will start with and brief overview of the DEEP architecture and the OmpSs programming model to motivate and contextualize the work presented. Then, the OmpSs offloading extensions to exploit heterogeneous cluster will be introduced and several examples will be used to illustrate how they work. The last part of the presentation will present a performance and scalability study done with an N-Body benchmark and a Full Waive Inversion application on Stampede and Marenostrum supercomputers respectively. [1] D. A. Mallon, N. Eicker, M. E. Innocenti, G. Lapenta, T. Lippert, and E. Suarez, “On the scalability of the clusters-booster concept: a critical assessment of the deep architecture”, in Proceedings of the Future HPC Systems: the Challenges of Power-Constrained Performance. ACM, 2012, p. 3. [2] F. Sainz, V. Beltran and J. Labarta, “OmpSs Collective Offload for Heterogeneous Clusters”, Submitted to the IEEE Cluster 2013 Conference, Chicago, Illinois, (USA), September 2015.

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Title: Feedback Control of Powder Mass Flow Rate in Laser Metal Deposition Processes

Author(s): Jennifer Bennett, Sarah Wolff, Kornel Ehmann, Jian Cao, *Northwestern U.*; Greg Hyatt, *DMG/Mori Seiki USA Inc*.

Maintaining uniform powder deposition per unit length in additive laser metal deposition processes is critical to achieving mechanical properties equivalent or superior to parts created by conventional processes. Control of powder mass flow is complicated by nonlinear effects due to carrier gas turbulence and low flow rates as well as significant material transport delays due to the nature of the powder feeder system. This paper proposes a novel approach to the regulation and control of the powder flow rate in laser metal deposition processes that eliminates complications induced by material transport delay. The powder flow will be regulated very near to the powder feeding nozzle, enabling the maintenance of uniform powder deposition per length even with disturbances in the motion system. This approach will encompass experimental validation of models that will take laser and powder feeding process parameters into account as well as molten powder morphology as feedback. The performance of the proposed control methodology will be evaluated by examining the mechanical properties, surface integrity and finish, size and prevalence of voids, and residual stress in finished parts.

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Title: Tied Contact for Explicit Dynamics with Isogeometric Analysis

Author(s): David Benson, *UCSD*; Attila Nagy, *LSTC*; Stefan Hartmann, *Dynamore*.

Tied contact is used to join meshes that do not have coincident control points or nodes, and is used in both traditional finite element analysis and isogeometric analysis (IGA). Tied contact may be imposed by either formulating constraints or with the penalty method. In general, constraints are preferred over the penalty method to exactly enforce the constraints and to eliminate any stability problems in explicit dynamics associated with a large penalty parameter. Using Lagrange multipliers to enforce the constraints in explicit dynamics is not cost effective since Lagrange multipliers require the solution of a system of linear equations. For traditional finite element formulations, the constraints may often be formulated in a manner that permits a local sequential solution that is efficient and robust because of the interpolatory nature of the basis functions. For IGA, where the basis functions are not interpolatory, the formulation of the constraints becomes more complicated. The issues associated with tied contact for IGA are explored here and preliminary results are presented.

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Title: Isogeometric Reduced-Order Modeling with Application to Optimization of Shells

Author(s): Joseph Benzaken, Christopher Coley, John Evans, *U. Colorado-Boulder*.

Isogeometric analysis was introduced in order to provide a direct link between geometric design and engineering analysis. However, the design of complex systems requires iteration as the design is adapted during the optimization process. In addition, solutions of complex multi-physics systems are expensive with respect to both storage and CPU costs. Reduced order models provide a way to quickly evaluate the solutions of these systems. This allows computational models to respond to changes in design geometry, and permits analysis of the effect of changes in design parameters at very little computational expense. To combine the relative strengths of isogeometric analysis and reduced order modeling, we introduce a new isogeometric reduced order modeling approach that leverages the emerging technology of sparse collocation. Our approach arises from the ability to define not just a single design geometry of interest, but rather a family of geometries in order to efficiently parametrize the design space for a given engineering system. Using sparse collocation, we are then able to sparsely sample this parametrized family to reliably predict system response over the complete design space. This new approach introduces a direct link between design and analysis for an entire class of geometries, and it further enables explicit and efficient computation of shape sensitivities with respect to geometric design parameters. In this talk, we present the basic theory underlying our reduced order modeling approach, and we demonstrate application to canonical shell structures of interest. Finally, we demonstrate the utility of our approach within the context of multi-objective shape optimization. In this context, we show that we can predict several quantities of interest simultaneously, and as our method does not require a priori specification of objectives or constraints, a user can easily modify optimality criteria without incurring additional computation.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Viscoplastic and Thixotropic Effects of Blood Rheology to Arterial Flow

Author(s): Antony Beris, Alex Apostolidis, John Fillenwarth, Adam Moyer, *U. Delaware*.

Antony N. Beris, Alex Apostolidis, John Fillenwarth and Adam Moyer Department of Chemical and Biomedical Engineering, University of Delaware, Newark, DE 19716, USA. Continuing our recent work on the viscoplastic [1] and thixotropic [2] characteristics of blood flow rheology, we present here an investigation of these effects in blood flow simulations within the human arterial network. First, this involves the implementation of a recently developed viscoplastic description of the steady-state blood flow rheology into the previously developed 1D model of the flow within the arterial network. This new rheological model is still based on the Casson equation but involves a new parameterization of its coefficients in terms of important physiological parameters, such as the blood hematocrit and fibrinogen concentration, so that it much better fits available experimental data [1]. A similar re-parameterization is also performed for the apparent Newtonian viscosity used in the description of the transient component of the flow. Second, it involves carrying out detailed, 3D and time-periodic, non-Newtonian blood flow simulations within a specific subsection of the coronary arterial network involving the first bifurcation of the left main coronary artery into the left circumflex (LCX) and left anterior descending (LAD) one. Following [3], the time-periodic blood flow simulations through the left main coronary, arterial bifurcation are carried out using a finite volume method implemented within a commercial 3D (FLUENT) code suitably adapted to allow for an efficient implementation of the proper (in vivo) outlet boundary conditions, as provided in the form of Fourier frequency impedance coefficients by the 1D model. In contrast to our previous simulations of the left coronary artery bifurcation [3], a much more faithful to the actual geometry mesh representation is used at this time, in addition to the implementation of non-Newtonian rheology characteristics both in FLUENT and in the 1D model (as described above). The non-Newtonian effects are examined in two cases: First in a healthy system, and second, in a diseased case where an occlusion has developed in one of the daughter vessels, resulting in strengthening the asymmetry of the bifurcation. References [1] Apostolidis, A.J., Beris, A.N, J. Rheol., 58(3): 607-633,(2014). [2] Apostolidis, A.J., Armstrong, M.J., Beris, A.N, J. Rheol., 59(1): 275-298,(2015). [3] Johnson, D.A., Naik, U.P., Beris, A.N., Int. J. Numer. Meth. Fluids, 66(11): 1383-1408, (2011). Acknowledgement This work is supported by NSF, Grant Award # NSF CBET 1033296.

13th U.S. National Congress on Computational Mechanics
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Title: Bulk Point Insertion Using a Smooth Frame Field for Hex-Dominant Meshing

Author(s): Paul-Emile Bernard, Jean-François Remacle, *U. catholique de Louvain*.

Hexahedral meshes are commonly preferred to tetrahedral meshes in engineering analysis. One of their main advantage resides in the fact that a lower number of elements is required for the same amount of vertices, compared to tetrahedra. Our purpose here is to develop a fully automated procedure for generating non uniform hex-dominant meshes that contain a maximum amount of hexahedra, both in volume and number. The main idea of the current approach is to decompose the meshing procedure in two different stages: first, bulk points are created inside the domain and are subsequently tetrahedralized; then, tetrahedra are recombined to create a mixed mesh containing a maximum amount of high-quality hexahedra. The recombination process can be seen as a maximum clique problem. Using graph theory, an algorithm to find the maximum clique is used to handle the open Schneider's pyramid problem, and is compared to a greedy recombination algorithm. The efficiency of the recombination process is known to significantly depend on the quality of the sampling of the vertices. A good vertex sampling depends itself on the quality of the underlying frame field that has been used to locate the vertices. Therefore, an iterative procedure to obtain a high quality three-dimensional frame field is presented. Initiating the frame field with the value of its nearest neighbor on the boundary, this procedure tends to reduce the impact of the geometric singularities on its neighborhood, while smoothing the frame field everywhere else. Finally, a new point insertion algorithm based on a frame field smoothness is developed. Points are inserted in priority in smooth frame field regions. The new approach is tested and compared with more frontal strategies on various geometries. We show that the new method leads to hex-dominant meshes exhibiting either an equivalent or a larger volume ratio of hexahedra (up to 20%) compared to the frontal point insertion approach.

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Title: Computational Studies of Strain-Induced Structural Transformations in 2D Transition Metal Dichalcogenides

Author(s): Joel Berry, Mikko Haataja, *Princeton U.*; Songsong Zhou, Jian Han, Shuyang Dai, David J. Srolovitz, *U. Pennsylvania*.

Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenide monolayers, exhibit a rich variety of electronic properties and novel 2D physics. There is currently great interest in developing new technologies based on these materials, for example, in ultrathin, flexible, nanoelectronic and optoelectronic devices. The ability to precisely tailor and manipulate the physical properties of 2D materials is therefore of fundamental scientific and technological interest. One means of doing so is through strain engineering, exploiting the fact that large and/or qualitative changes in electronic transport properties can be readily induced with appropriate mechanical strains. For example, recent work on MoS2 and related transition metal dichalcogenides suggests that it is possible to exploit strain-induced structural transformations to rapidly switch between crystal structures that are semiconducting and metallic. We have constructed a mesoscale continuum model based on the phase field microelasticity (PFM) approach to describe such displacive transformations in these systems. The model incorporates the effects of transformation strains, domain boundaries between the symmetryrelated orientational variants of the transformed phase, long-range elastic interactions between domains, and coupling to applied stress or strain. Density functional theory (DFT) calculations of atomistic domain boundary structure and energetics are employed to guide development of the coarse-grained PFM description and to provide quantitative input parameters related to defect/ interfacial energetics. Simulation results for both substrate-supported quasi-2D monolayers and suspended monolayers that can deform out of the 2D plane will be discussed, and issues of transformation reversibility and recoverability will be explored. This work was supported as part of the Center for Computational Design of Functional Layered Materials (CCDM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

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Title: Multi-Scale Multiphysics Simulations at Extreme Scale Using Uintah

Author(s): Martin Berzins, *U. Utah*.

The challenge of computing the solutions to a number challenging engineering problems at extreme scale using the Uintah code is described. The Uintah code with its layered task-based and runtine-execution approach makes it possible solve problems at large scale without severe demands on the engineering users. A number of success stories are described and the challeges of modeling radiation in a large clean-coal combustion problem described. Results are shown from Titan and Mira to demonstrate the effectiveness of the Uintah software approach of usiong asynchromous adaptive task-based runtime systems.

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Title: Experimentally Validated Multi-Scale Modeling of the Dynamic Response of Composite Materials

Author(s): Miguel Bessa, Wing Kam Liu, *Northwestern U.*; Xiaoming Bai, L. Guo, *Harbin Inst. Tech.*; Antonio Melro, Pedro Camanho, *U. Porto*.

There is an increasing demand for accurate predictive models of the inelastic and fracture behavior of fiber reinforced polymer matrix composites due to the wide spread of applications where these materials are being used, especially in the transportation industry. However, accurately modeling the visco-thermo-mechanical behavior of these materials remains a difficult challenge due to various factors, namely: 1) the matrix material is usually a highly cross-linked glassy polymer (e.g. epoxy resin) that shows rate- and thermal-dependent inelastic response; 2) the fiber distribution is non-uniform; 3) the high strength and brittleness of the fibers associated to the high fiber volume fraction of the composite leads to large three-dimensional strain concentrations in the matrix; 4) the interface between fibers and matrix and/or the interphase region may affect significantly the response of the composite; and 5) the manufacturing process introduces thermal residual stresses and different defects such as voids, fiber waviness and fiber misalignment. These factors limit the applicability of analysis models based on the homogenized behavior of the composite. The work presented herein introduces a newly developed multi-scale model for the dynamic response of polymer matrix composites. A high-fidelity micromechanical model for the composite was developed where one of the key innovations resides in the plasticity model for the polymeric matrix that is based on the homogenization of nano-scale simulations. The obtained continuum visco-thermo-plastic model was experimentally validated for different load cases at different strain-rates and temperatures. Different representative volume elements for the composite were developed to predict the response of the material and good agreement with the experimental results was observed. To the authors' knowledge, this is the first multi-scale model for composite materials that is fully experimentally validated at each of the different scales. Finally, a new homogenization technique is proposed based on an image processing algorithm that is believed to be a viable alternative to the current homogenization techniques. A proof of concept demonstration of the method will be shown.

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Title: An Adaptive and Implicit Immersed Boundary Method for Cardiovascular Device Modeling

Author(s): Amneet Pal Singh Bhalla, *U. North Carolina-Chapel Hill*; Boyce Griffith, *U. North Carolina-Chapel Hill*.

Computer models and numerical simulations are playing an increasingly important role in understanding the mechanics of fluid-structure interactions (FSI) in cardiovascular devices such as artificial heart valves (bioprosthetic or mechanical) and pulse duplicator based valve testing machines. Such simulations expedite both the design process of cardiac devices, as well as help them to get approved from regulators. To model cardiac devices realistically, there is a need to solve the classical fluid-structure interaction equations efficiently. Peskin's explicit immersed boundary method is one such approach to model FSI equations for elastic structures efficiently that makes use of structured Cartesian grid solvers even for structures with complex geometries. However, in the presence of rigid structures (which are ubiquitous in cardiac devices) the classical IB method faces a severe timestep restriction. To overcome this limitation, we are developing an implicit version of immersed boundary method on adaptive Cartesian grids. Higher grid resolution is employed in spatial regions occupying the structure while relatively coarser discretization is used elsewhere in the computational domain. The resulting discrete system is solved using geometric multigrid solver for the combined Stokes and elasticity operators. We use a rediscretization approach for standard finite difference approximations to the divergence, gradient, and viscous stress. In contrast, coarse grid versions of the Eulerian elasticity operator are constructed via a Galerkin approach. The implicit IB method is tested for a pulse duplicator cardiac device system that consists of both rigid mountings and an elastic membrane.

13th U.S. National Congress on Computational Mechanics
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Title: A Numerical Study for the Effect of Vegetative Canopy on Turbulent Transport of Pollutants

Author(s): Md Abdus samad Bhuiyan, Jahrul Alam, *Memorial U.*.

Analyzing the mechanisms that influence scalar dispersion in the Earth's atmosphere is critical for several applications. For instance, turbulent transport of plant pathogens is a primary vehicle that spread many disease epidemics. Accurate prediction and scaling of turbulent flow past a canopy is useful to mitigate the growing threat of air pollution. Since the canopy flows are characterized by heterogeneity, intermittency, and non-Gaussian flow statistics, accustomed turbulence modeling approaches are not pertinent. Classical models are based on the assumption that a turbulent flow can be decomposed into a coherent structure and a chaotic component. Nonetheless, canopy turbulence is superimposed with a background shear flow, Earth's rotation, and mixed layer stratification. In this talk, I will present a simplified numerical methodology that extends the Deslauriers-Dubuc subdivision scheme for simulating flow past a canopy using the Navier-Stoke equation. I will discuss how the canopy is parameterized within this numerical model. Nevertheless, a primary focus of this talk aims to demonstrate the performance of the canopy flow solver. Some validation results will be presented.

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Title: Adaptive Spectral Tensor-Train Decomposition for Uncertainty Quantification

Author(s): Daniele Bigoni, Allan Engsig-Karup, *Tech'l. U. Denmark*; Youssef Marzouk, *MIT*.

We present a new method for the efficient and adaptive approximation of high-dimensional functions, in the context of uncertainty quantification. The method is based on the spectral tensor-train (STT) decomposition [1], which combines low-rank approximations in tensor-train (TT) format [2] with univariate polynomial approximations, leading to fast spectral convergence on functions with sufficient regularity. To construct an approximation of fixed polynomial degree, the TT-DMRG-cross sampling method [3] is used on the "quantics" folding of the tensor resulting from an appropriate discretization of the target function; the resulting number of function evaluations scales linearly with the parameter dimension and quadratically with the TT ranks. A reweighing of the TT construction ties the accuracy of the cross-interpolation to the L^2 error of the function approximation, rather than the Frobenius norm of the discrete tensor. We then derive an a posteriori error estimator that enables anisotropic adaptation of the polynomial approximation space, and construct the associated STT approximations with the help of heuristics to select starting points for the optimization algorithm TT-DMRG-cross. We investigate adaptive tensor discretizations based on either Gaussian or nested quadrature rules. We demonstrate the performance of these approximations on both synthetic functions and real applications of uncertainty quantification. Overall, the adaptive STT construction allows an incremental assembly of the approximation, avoiding the need to pre-select the polynomial degree and allowing more control over the trade-off between computational effort and accuracy. [1] Bigoni, D., Engsig-Karup, A. P., & Marzouk, Y. M. (2015). "Spectral tensor-train decomposition." arXiv:1405.5713 [2] Oseledets, I. V. (2011). "Tensor-train decomposition." SIAM Journal on Scientific Computing, 33(5), 2295–2317. doi:10.1137/090752286 [3] Savostyanov, D., & Oseledets, I. (2011). Fast adaptive interpolation of multi-dimensional arrays in tensor train format. The 2011 International Workshop on Multidimensional (nD) Systems, 1–8. doi:10.1109/nDS.2011.6076873

13th U.S. National Congress on Computational Mechanics
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Title: High-Dimensional Uncertainty Propagation via a Bayesian Gradient-Free Reformulation of Active Subspace Methodologies

Author(s): Ilias Bilionis, Rohit Tripathy, Marcial Gonzalez, *Purdue U.*.

Uncertainty propagation (UP) in high-dimensions is an exponentially hard problem. The number of dimensions that can be treated varies depending on the technique employed and on the smoothness of the response surface. To give some indicative numbers, consider that generalized polynomial chaos (gPC) blows up at around 10 stochastic dimensions, Gaussian process regression (GPR) encounters problems at around 20 stochastic dimensions, adaptive sparse grid collocation (ASGC) can deal with up to 50-70 dimensions, and high-dimensional model representation (HDMR) has been shown to work with up to a few hundreds, if only the very first terms of the expansion are retained. Note that these numbers refer to ideal cases of relatively smooth responses, and that for arbitrary situations performance will quickly degrade with increasing stochastic dimensions. The curse of dimensionality can be addressed only if the response exhibits special structure that can be discovered and exploited. It is an empirical fact, evidence of which we are going to provide, that a wide array of physical responses exhibits a special structure known as an active subspace (AS). An AS is a manifold of the stochastic space characterized by maximal response variation. The idea is that one should first identify this low dimensional manifold, and then learn the map between it and the response. Sate-of-the-art methodologies discover AS's using gradient information, a fact that severely limits the applicability of the method. We propose a Bayesian reformulation of AS that relies on a new covariance function for GPR with build-in dimensionality reduction. It does not require gradient information, a fact that makes it applicable to a wider range of applications. Instead, it infers the projection matrix by maximizing the likelihood over a Stiefel manifold. The number of active dimensions is also inferred systematically. Finally, we discuss two possible extensions of AS that target 1) multi-output responses using q-dimensional Gaussian processes (GP) and 2) identifying non-linear active manifolds using mixtures of GP's. We demonstrate our approach on problems with hundreds of stochastic dimensions. Specifically, we study the propagation of compact solitary waves in granular crystals, or arrays of elastic spherical particles in contact. A systematic study of all sources of uncertainty (such as material properties and geometric parameters) and their impact on the unique wave dynamics of these strongly nonlinear systems has never been done before.

13th U.S. National Congress on Computational Mechanics
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Title: Scalable Algorithms for Kernel Sums in Computational Physics and Statistical Inference

Author(s): George Biros, *UT Austin*.

Kernel sums are the computational cornerstone for many problems in mathematical physics. The are equivalent to dense matrix multiplications and as such, they have quadratic complexity. For scalable algorithms, the basic challenges are overcoming the quadratic complexity for matrix vector multiplication operator. There are three basic approaches to overcome this barrier. Nearest-Neighbor approximations, global low-rank approximations, and N-body algorithms. The latter can be modified to include both nearest-neighbor and global low-rank approximations. In this talk, I will present (1) a brief history of N-body algorithms and their application to multiscale problems; (2) give a brief overview of the most basic N-body algorithm, the Barnes-Hut method; (3) expand the notion of N-body problems to high-dimensional problems and statistical inference; (4) conclude with applications of N-body algorithms to physics (fluid mechanics) and statistics (supervised learning).

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Title: Variational Methods for Consistent Mass Scaling and Direct Construction of Inverse Mass Matrices

Author(s): Anne-Kathrin Schaeuble, Anton Tkachuk, Manfred Bischoff, *U. Stuttgart*.

Mass scaling is often applied in explicit dynamic finite element analysis with the aim of increasing the critical time step. The concept relies on reducing the highest frequencies of a discrete system while retaining the lowest modes, thus avoiding significant loss of accuracy. In contrast to algebraic mass scaling techniques [1] the recently proposed technology of variational selective mass scaling [2] allows the systematic design of consistent scaled mass matrices. The method is based on a parameterized multi-field Hamilton's principle, inspired by Felippa's work on parameterized variational principles. The variational framework allows designing new mass scaling schemes with particular features, depending on the choice of certain parameters. It also provides a mathematical justification of existing methods for selective mass scaling. Owing to the variational background, consistency and thus convergence is intrinsically guaranteed. Like in algebraic selective mass scaling, translational and rotational inertia may be preserved. It is also possible to construct consistent singular mass matrices which can be useful in implicit analysis of contact and impact problems. Both algebraic and variational mass scaling increase computational expense for each individual time step, because, in contrast to a lumped mass matrix, inversion of the mass matrix is not trivial and a linear system of equations has to be solved within each explicit time step. Nevertheless, due to the increased critical time step, the overall computation time is usually reduced. Moreover, the aforementioned variational framework also allows a direct construction of sparse inverse mass matrices [3], thus being computationally as efficient as mass lumping. Depending on the application this new technology may considerably outperform selective mass scaling techniques based on algebraic constructions. Performance of the method is investigated by means of dispersion analyses and it is demonstrated by numerical examples. Applications to standard and isogeometric finite elements are presented. References [1] L. Olovsson, K. Simonsson, M. Unosson. Selective mass scaling for explicit finite element analyses. Int J Numer Methods Eng 63, 1436-1445, 2005. [2] A. Tkachuk, M. Bischoff, Variational methods for selective mass scaling. Comp Mech. 52, pp. 563-570, 2013. [3] A. Tkachuk, M. Bischoff. Direct and sparse construction of consistent inverse mass matrices: general variational formulation and application to selective mass scaling. Int. J. Num. Meth. Engng. 101, pp. 435–469, 2015.

13th U.S. National Congress on Computational Mechanics
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Title: Direct Numerical Simulations in Solid Mechanics for Quantifying the Effects of Microstructure and Material-Model Form Error on Macroscale Quantities of Interest

Author(s): Joseph Bishop, John Emery, Corbett Battaile, *Sandia Nat'l. Lab.*.

Two fundamental sources of error in macroscale solid-mechanics modeling are (1) the assumption of scale separation in homogenization theory and (2) the use of a macroscopic material model that attempts to represent, in an average sense, the complex nonlinear processes occurring at the microscale. In an era of petascale computing, and with the promise of future exascale computing, it is now possible to perform direct numerical simulations (DNS) in solid mechanics where the microstructure is modeled directly in a macroscale structure. Using this DNS computational capability, we perform direct numerical simulations in which polycrystalline microstructures are embedded throughout a macroscale structure. The structural material is austenitic 304L stainless steel, and a crystal-plasticity constitutive model is used to model the elastic-plastic response within each grain. The DNS simulations are compared to a conventional macroscale simulation that assumes a homogenized elastic-plastic response modeled with a standard J2-plasticity model. Detailed comparisons are made in both macroscopic and microscopic quantities of interest for a range of loading conditions, both proportional and nonproportional.

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Title: High-Performance Semilocal Transient Algorithms for the High-Order FEM

Author(s): Marco Bittencourt, Gilberto Valente, *U. Campinas*.

Local and semilocal explicit and implicit algorithms were developed in [1,2] and applied to linear elasticity and fluid-solid-interaction problems. The main idea is to solve the system of equations for each element and obtain the global solution using a least square method. Due to the global nature of the boundary conditions, the solution of a residue equation is required by an iterative method. In this work we will apply these algorithms to linear elastic problems in the Blue Gene computer to solve very large hog-order meshes. Minimum energy bases will be used to solve the residue equation due to their low conditions numbers for high-order interpolation. The similarity with the balancing domain decomposition method will be presented. [1] M.L. Bittencourt; F.A. Furlan. An elementwise least square approach for explicit integration methods applied to elas- ticity. MecSol 2011 – International Symposium on Solid Mechanics, 2011, Florianopolis. Solid Mechanics in Brazil 2011, Florianópolis, Santa Catarina, Brasil, 2011; 63–76. [2] Y., Yue; M.L. Bittencourt; G.E. Karniadakis. A semi-local spectral/hp element solver for linear elasticity problems. International Journal for Numerical Methods in Engineering, 100 (5), 347-373, 2014.

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Title: Proportional Topology Optimization: A New Non-Sensitivity Method for Solving Stress Constrained and Minimum Compliance Problems and Its Implementation in MATLAB

Author(s): Emre Biyikli, Lin Cheng, Albert To, *U. Pittsburgh*.

Topology optimization is recently getting more attention due to the recent advancement of additive manufacturing since it facilitates the manufacture of porous structural designs with arbitrarily-complex geometries so that higher strength-to-weight ratios can be attained [1]. A new topology optimization method called the Proportional Topology Optimization (PTO) is presented to solve the stress constrained and minimum compliance problems. In the PTO algorithm, the design variable (e.g. density) is distributed to each element in the finite element model in proportional to its stress (or compliance) over the global sum of the stress (or compliance) values in every iteration step. This global approach of the PTO is different from the full stress design (FSD) which utilizes a strictly element-wise approach [2]. As a non-sensitivity method, PTO is simple to understand, easy to implement, and is also efficient and accurate at the same time. It is implemented into two MATLAB programs to solve the stress constrained and minimum compliance problems. Descriptions of the algorithm and computer programs are provided in detail. The method is applied to solve three numerical examples for both types of problems. The method shows comparable efficiency and accuracy with an existing optimality criteria method which computes sensitivities [3]. Also, the PTO stress constrained and minimum compliance algorithms are compared by feeding output from one algorithm to the other in an alternative manner, where the former yields lower maximum stress and volume fraction but higher compliance. Advantages and disadvantages of the method and future works are discussed. The computer programs are self-contained and publicly shared in the website www.ptomethod.org. [1] P. Zhang, J. Toman, Y. Yu, E. Biyikli, M. Kirca, M. Chmielus, A.C. To, Efficient Design-Optimization of Variable-Density Hexagonal Cellular Structure by Additive Manufacturing: Theory and Validation, Journal of Manufacturing Science and Engineering, (2014). [2] R.T. Haftka, Elements of structural optimization, Springer, 1992. [3] E. Andreassen, A. Clausen, M. Schevenels, B.S. Lazarov, O. Sigmund, Efficient topology optimization in MATLAB using 88 lines of code, Structural and Multidisciplinary Optimization, 43 (2011) 1-16.

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Title: Pipe-Oriented Finite Elements for the Three-Dimensional Blood Flow Simulation

Author(s): Alonso Alvarez, Pablo Blanco, Raúl Feijóo, *Nat'l. Lab. Scientific Computing, Brazil*.

In the current years, rather sophisticated function bases are being under scrutiny to reduce computational cost at the expense of adding off-line complexity either in the coding stage or in the pre-processing part of a simulation. In the modeling of blood flow in arterial vessels, domains of analysis have a very specific characteristic: they are an arrangement of branching pipes. Taking advantage of this a priori knowledge allows practitioners to find a trade-off solution between costly three-dimensional finite element simulations and extremely simplified one-dimensional approximations of blood flow. In the previous context, and inspired in the ideas behind the hierarchical modeling technique [1,2,3], in this work we explore numerically the capabilities of two very peculiar families of high order finite elements: (i) a Cartesian finite element and (ii) a Cylindrical finite element in the simulation of fluid flow phenomena. These two families feature a low order approximation in the axial direction (dominant direction of fluid flow phenomena), and a high order approximation in the cross-sectional section. Issues related to bifurcations in three-dimensional space will be discussed and challenges will be identified. Numerical results will be presented in cases with flow regime similar to those encountered in arteries, including comparisons against classical finite element simulations. [1] S. Perotto, A. Ern and A. Veneziani. Hierarchical local model reduction for elliptic problems: a domain decomposition approach. Multiscale Model. Simul., 8 (2010), 4, 1102-1127. [2] Matteo Carlo Maria Aletti. Educated bases for HIerarchical MODel reduction in 2D and 3D. Mathematical Engineering Degree, Politecnico di Milano, 2013. [3] Sofia Guzzetti. Hierarchical model reduction for incompressible flows in cylindrical domains. Mathematical Engineering Degree, Politecnico di Milano, 2014.

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Title: Least Squares Shadowing: A Sensitivity Analysis Method for Chaotic and Turbulent Fluid Flows

Author(s): Patrick Blonigan, Qiqi Wang, *MIT* .

Computational methods for sensitivity analysis are invaluable tools for aerodynamics research and engineering design. These tools, including the adjoint method, make the optimization of aerodynamic shapes with many design parameters feasible. Sensitivity analysis is used in many other applications as well, including error estimation, adaptive grid refinement, uncertainty quantification, and flow control. However, traditional sensitivity analysis methods break down when applied to long-time averaged quantities in chaotic fluid flow fields (Lea, 2000), such as those obtained using high-fidelity turbulence simulations including DES and LES. As most key scientific and engineering quantities of interest in turbulent flows are long-time averaged quantities, finding methods to compute their sensitivities will push the frontiers of aerodynamic design. However, a number of dynamical properties of chaotic fluid flows, most importantly Edward Lorenz's ``Butterfly Effect'', make the formulation of robust and efficient sensitivity analysis methods difficult. A new sensitivity analysis method developed by the authors, Least Squares Shadowing (LSS), can compute useful and accurate gradients for quantities of interest in chaotic and turbulent fluid flows (Wang, 2014). LSS computes gradients using the ``shadow trajectory'', a phase space trajectory (or solution) for which perturbations to the flow field do not grow exponentially in time. The shadow trajectory is computed by solving a least squares minimization problem, hence the name “Least Squares” Shadowing. This talk first discusses the reasons for the break down of conventional sensitivity analysis methods for chaotic flow fields. This break down is illustrated a number of examples, including the Lorenz Attractor, and an airfoil at a high angle of attack. All of these cases are highly sensitive to initial conditions and any small perturbation to the flow field will eventually result in drastic changes. The talk will go on to outline the theory behind LSS and how it is implemented in practice. LSS is then demonstrated on a few chaotic and turbulent fluid flows, including homogeneous isotropic turbulence and a stalled airfoil. References: Lea, D., Allen, M., and Haine, T., “Sensitivity analysis of the climate of a chaotic system,'' Tellus, Vol. 52A, 2000, pp. 523-532. Wang, Q., Hui, R., and Blonigan, P., “Least Squares Shadowing sensitivity analysis of chaotic limit cycle oscillations,'' Journal of Computational Physics, Vol. 267, June 2014, pp. 210-224.

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Title: On a Challenge Prof. Ted Belytschko Announced at USNCCM 1999 Boulder, CO

Author(s): Florin Bobaru, *U. Nebraska-Lincoln*.

I vividly recall Prof. Ted Belytschko's plenary lecture at the US National Congress on Computational Mechanics in Boulder, Colorado from 1999. This was one of the first major conferences I was participating at. It was on this occasion that my Ph.D. advisor at Cornell, Prof. Subrata Mukherjee, introduced me to Prof. Belytschko. In my Ph.D. thesis I had used Ted's Element-free Galerkin (EFG) method in shape optimization problems. Perhaps the most important lesson I learned during that memorable USNCCM, beside the need to carry another pair of shoes in case a 45 minute rain downpour hits just before the congress banquet, was from Prof. Ted Belytschko's plenary lecture. In his unique style of presentation, combining witty remarks with sharp observations and jokes, I recall the challenge Prof. Belytschko addressed to the young researchers in the audience. Paraphrasing from memory now, my recollection is that prof. Belytschko's message for the next generation of researchers in computational mechanics was: "do not be afraid to attack the difficult problems in computational mechanics, the nonlinear problems (among which he cited dynamic fracture); do not try to "play-it-safe", take risks in trying to solve tough problems!". A few years after the 1999 USNCCM, I happened to start working on dynamic fracture problems. In this presentation I will give an account of the progress we made in understanding this complex, nonlinear phenomenon in brittle materials. I will discuss the crack branching problem in brittle materials, which is a dynamic effect that precedes, for example, fragmentation. I will then present results for impact damage/fragmentation in brittle targets. I will give motivations for using a nonlocal model, peridynamics, in solving such problems. This talk is dedicated to the memory of Professor Ted Belytschko, who has inspired entire generations of researchers in computational mechanics.

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Title: Efficient and Robust Usage of CAD Parameterization Capability for Aerodynamic Shape Optimization

Author(s): Kamil Bobrowski, *U. Politecnica Madrid*; Holger Barnewitz, *AIRBUS Operations*.

Designing aerodynamic shape of the aircraft is a complex sequential process, requiring multidisciplinary approach, which impose various constraints on the possible shapes. Moreover, many current developments are focused on improving existing aircrafts, thus the design space is further reduced. The target is to search for the optimal aerodynamic shape in the field of acceptable structure modifications. Accurate shape, subject to geometrical constrains, can be obtained through Computer Aided Design (CAD) software, thus creating a link between the CAD geometry and the CFD surface mesh is essential. This paper presents a novel approach for linking shape deformation in CAD software and CFD mesh deformation. The core idea is to utilize a geometry surrogate model of the discrete surface deformation field extracted from parametric CAD surface. For given values of design parameters the surrogate model provides fast and robust prediction of the deformation field, which is used as an input for CFD mesh deformation. RANS flow equations can be solved on the deformed mesh. With this process in a loop, an optimization algorithm is used, which leads to an optimum in the space of feasible shape modifications. Added value of this method is that CAD software is used only for the geometry surrogate model creation, and is not called during the optimization. Subsequent steps of the proposed process are described, including a new method to capture discrete shape deformation in CAD program, creation of the geometry surrogate model based on Proper Orthogonal Decomposition (POD), mesh deformation, and CFD optimization using both gradient-based and surrogate-based methods. To assess performance and usability of this modern approach two test cases have been selected and described in this paper: medium-size problem (twist optimization of transonic wing) and full-size industrial test case. In both cases the method proved to accurately predict the discrete deformation field for given values of design parameters with a negligible time effort. The optimization process has been significantly simplified by eliminating calls to CAD software inside the loop. Although this process was developed for aerodynamic shape optimization, it can be used in any application which requires robust and computationally cheap method for handling the design space of CAD-based shape modifications.

13th U.S. National Congress on Computational Mechanics
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Title: A Variational Flux Recovery Approach for Elastodynamics Problems with Interfaces

Author(s): Pavel Bochev, Paul Kuberry, *Sandia Nat'l. Lab.*.

We present a new explicit algorithm for linear elastodynamic problems with material interfaces. The method discretizes the governing equations independently on each material subdomain and then connects them by exchanging forces and masses across the material interface. Variational flux recovery techniques provide the force and mass approximations. The new algorithm has attractive computational properties. It allows different discretizations on each material subdomain and enables partitioned solution of the discretized equations. The method passes a linear patch test and recovers the solution of a monolithic discretization of the governing equations when interface grids match.

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Title: The Finite Element Immersed Boundary Method with Distributed Lagrange Multiplier

Author(s): Daniele Boffi, *U. Pavia, Italy*.

In this talk we review recent results, obtained in collaboration with Nicola Cavallini and Lucia Gastaldi, related to the finite element immersed boundary method (FE-IBM) for the approximation of fluid-structure interaction problems. In [1] we consider a modification of the original FE-IBM based on the introduction of a Lagrange multiplier. More precisely, the ordinary differential equation which governs the motion of the solid is reformulated in a variational form, which at the same time offers more flexibility to the numerical scheme and is more natural in the framework of finite element discretization. Our new formulation can be considered as a specific case of a fictitious domain approach with distributed Lagrange multiplier and for this reason we refer to it as DLM-IBM. Our DLM-IBM formulation is different from previous investigations based on a DLM approach, since our structure has a viscoelastic nature. We propose a numerical approximation of the DLM-IBM formulation based on a semi-implicit time advancing scheme. Theoretical results show that the scheme is unconditionally stable with respect to the time step size (no restriction at all on the time step). Preliminary numerical tests show optimal convergence in time and space as well as unexpectedly superior mass conservation. [1] D. Boffi, N. Cavallini, and L. Gastaldi. The Finite Element Immersed Boundary Method with Distributed Lagrange multiplier. arXiv preprint 1407.5184

13th U.S. National Congress on Computational Mechanics
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Title: The Effect of Microstructural Heterogeneity on Ductile Fracture

Author(s): Geoffrey Bomarito, James Warner, *NASA*.

Ductile fracture is a material failure mechanism which occurs by the growth and coalescence of micro-scale voids. Despite the heterogeneous microstructure that nucleates these voids, most common ductile fracture models assume a uniform value of initial porosity. In this work, a multi-scale model is introduced that describes the uncertainty in ductile fracture initiation due to spatial heterogeneity at the micro-scale. First, several micro-scale 3-D finite element (FE) models, corresponding to many initial porosities, are subjected to a suite of loading cases. The results of these simulations are used to calibrate a continuum-scale material model which effectively defines the response of the material as a function of loading and local initial porosity. Because the continuum-scale model accounts for initial porosity, it can be applied to a component scale model in which the spatial distribution of initial porosity is non-constant. Accordingly, several component-scale FE models are built using the continuum-scale response, each with heterogeneously distributed initial porosities. The result is a Monte Carlo based description of the distribution of ductile fracture initiation in a given test specimen. The distribution is compared to experimental data as well as two homogenization approaches.

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Title: The Mechanical Behaviour of New Hybrid Sandwich Structures Based on Corrugated-Core and Fibre Metal Laminates Under Low-Velocity Impact Loading

Author(s): Tawan Boonkong, Zhongwei Guan, ALIA RUZANNA AZIZ, *U. Liverpool*; Wesley James Cantwell, *Khalifa U. Sci., Tech. & Rsch.*.

A series of experimental investigations and numerical analyses is presented into the impact response, and subsequent failure modes in a new hybrid sandwich structure based on corrugated-core and fibre metal laminates. The new hybrid sandwich structure was produced by a combination of Glass Laminate Aluminium Reinforced Epoxy (GLARE) and corrugated-core, using a hot press moulding technique and then bonded to face sheets based on the prepreg of glass fibre, to produce a range of lightweight sandwich panels. The low velocity impact tests were carried out to investigate the role of core thickness, corrugated core configurations, and change materials. The experiments also provide an insight into the post-failure response of the sandwich panels. The Abaqus/explicit software package was used and the finite element modelling was developed by using cohesive elements, elasto-plastic with strain hardening, rate dependent and damage criteria such as Hashin's damage for composite materials, ductile and shear damage, and also buckling mode. Simulations of compressive characteristics of the new hybrid sandwich structures were presented, which were validated against the corresponding experimental data. The predictions of the simulation of the new hybrid sandwich structure generally in a good agreement with the experimental results. Finally, the specific energy absorption properties of the new hybrid sandwich structures are compared to the other core materials where evidence suggests that these systems compare favourably with their more conventional counterparts.

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Title: Point Collocation Methods for Free Boundary Problems

Author(s): Stephane Bordas, Satyendra Tomar, *U. Luxembourg, Cardiff U.*; Xuan Peng, P. Kerfriden, *Cardiff U.*; George Bourantas, *U. Luxembourg*; Elena Atroshchenko, *U. Chile*; Karol Miller, *U. Western Australia*.

This talk presents recent advances in the development of IGA-based and meshless-based point collocation techniques for problems involving free boundaries, both in solid and fluid mechanics, with applications ranging from smart fluids and active matter to biomechanics. We present recent results in (1) isogeometric boundary element methods for damage tolerance assessment directly from CAD; (2) the simulation of mantle convection and nematic liquid crystals using meshless point collocation approaches based on a DC-PSE approximation scheme. We show in particular that, provided suitable integration schemes are used, the isogeometric boundary element method we propose enables the simulation of fracture directly from CAD data, and that the DC-PSE operators provide stable meshless point collocation methods for both solid and fluid mechanics.

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Title: The Variational Approach to Fracture and Ductile Materials

Author(s): Michael Borden, Eric Domonell, *North Carolina State U.*.

In this presentation, we will describe our recent efforts to extend the variational approach to fracture to the prediction of dynamic fracture in ductile materials. The variational approach to fracture was originally introduced in the context of Griffith's theory for brittle fracture and results have shown that this approach can accurately predict crack growth in brittle material. Initial attempts to extend the theory to ductile materials have recently appeared in the literature but there is still much to do. We will present our recent work to apply the variational approach to fracture to ductile materials. We will also discuss our development of the constitutive theory for phase-field models of ductile fracture and present several numerical examples for both two- and three-dimensional problems with comparisons to experimental results. These examples will demonstrate the ability of phase-field models to accurately capture complex crack propagation patterns in ductile materials.

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Title: Computational Modeling of Micro-Fracture Processes Triggering Shear Band Bifurcation in Porous Crystalline Rocks

Author(s): Martin Tjioe, Ronaldo Borja, *Stanford U.*.

We develop a computational framework that captures the micro-fracture processes triggering shear band bifurcation in porous crystalline rocks. The framework consists of computational homogenization on a representative elementary volume (REV) that upscales the pore-scale micro-fracture processes to the continuum scale. The assumed enhanced strain (AES) finite element approach is used to capture the discontinuous displacement field generated by the micro-fractures. Homogenization at the continuum scale results in incrementally nonlinear material response, in which the overall constitutive tangent tensor varies with the stress state as well as with the loading direction. Continuum bifurcation detects the formation of a shear band on the REV level; 3D strain probes, necessitated by the incremental nonlinearity of the overall constitutive response, determine the most critical orientation for shear band bifurcation. Numerical simulations focus on micro-fracturing at the pore scale with either predominant interface separation or predominant interface contact modes. Results suggest a non-associative overall plastic flow and shear band bifurcation on the rising part of the overall stress-strain response.

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Title: A Scalar Limiting Algorithm for High-Order Methods

Author(s): Eurielle Bossennec, Guido Lodato, Luc Vervisch, *Normandie U., CNRS, INSA, U. Rouen*.

High-order methods have gained in interest over the past decade for their ability to represent the flow characteristics and physics with better accuracy than classical low-order methods would allow, also because they introduce very little numerical dissipation. However, this feature makes them more prone to develop non-physical oscillations of the solution (overshoots, undershoots and wiggles) in regions of strong gradients. This issue has already been addressed in different ways (slope limiters, positivity-preserving schemes, additional viscosities, etc.), mostly in the context of high-speed flows with shocks where density, velocity and pressure need to be limited close to discontinuities. The code adopted in this study, originally developed at Stanford by Antony Jameson's group, is based on the high-order spectral difference method, a discontinuous finite-element scheme for unstructured hexahedral meshes. This scheme shares most of the features of the the discontinuous Galerkin method while being relatively simplier to implement. A shock-capturing method based on the use of a modal sensor to detect discontinuities is already implemented and working successfully for flows with shocks [2]. Focusing on turbulent combustion applications, computations involving reactive or non-reactive scalar transport are performed, where the scalar boundedness has to be preserved (e.g. mass fractions or progress variables which have to be strictly bounded between 0 et 1). To do so, the shock capturing method previously mentioned is adapted to sense scalar overshoots/undershoots and to introduce the required dissipation to guarantee boundedness. Auto-calibration of the sensor and the relevant additional artificial viscosity is also implemented. This methodology as well as the skyline pessimization method introduced by Klöckner et al. [1] are tested over simple classical testcases, namely a 1D Heaviside function convected at M = 0.01 and 2D circular convection of a given profile, proposed by Waterson [3]. In both cases, the proposed method is successfully validated, the scalar being bounded within less than 0.1% for different mesh resolutions and polynomial orders. The approach will be further tested in more complex configurations such as a 3D turbulent jet, first in a non-reactive case, next in a reactive flow. [1] Klöckner, Warburton, Hesthaven 2011. Math.Model.Nat.Phenom. 2011-6. [2] Persson, Peraire 2006. AIAA P. 2006-112. [3] Waterson, Deconink 2007. J.Comput.Phys. 2007-224.

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Title: Microstructure Characterization and Reconstruction: A Supervised Learning Approach

Author(s): Ramin Bostanabad, Wei Chen, *Northwestern U.* ; Anh Bui, Daniel Apley, *Northwestern U.*; Wei Xie, *RPI*.

Characterization and Reconstruction are indispensable parts of computational materials science. This is in large part due to either avoiding to conduct physical experiments on the original sample or taking into account the inherent uncertainty associated with material behavior. The main contribution of this work is to introduce, for the first time to the researchers' best knowledge, a supervised learning approach for characterization and reconstruction of a broad range of random heterogeneous microstructures. We presume the microstructure is Markovian and then, building on the consequent locality and stationarity assumptions, convert its digitized image into a set of training data. Afterwards, we use a supervised learner, a classification tree, to fit a flexible and interpretable model to the high dimensional data in order to characterize the conditional distribution of material constituents. Once the model is fitted, it can be used to efficiently build an ensemble of statistically equivalent microstructures that can be used for property evaluation and prediction (for instance via Finite Element Analysis). Our model is either Causal or Non-Causal with, respectively, single-pass and multi-pass reconstruction schemes. We reconstruct a statistically equivalent microstructure pixel by pixel in a raster scan order by predicting the probability of having a particular material state at a location and, subsequently, feeding that probability into a multinomial random variable. We test the approach on various case studies and evaluate the results via two-point and two-point cluster correlation functions to show that the spatial dependencies within the microstructure are well preserved. The main superiority of our approach lies in having a model that not only makes the reconstruction process computationally more efficient than other methods (esp. optimization–based ones), but also can be used for design and inspection purposes. The methodology is completely data-driven and standalone since only the information embedded in the microstructure are used. The limitations of the Supervised Learning approach arise from the two key assumptions made in its development: Locality and Stationarity. If the original microstructure does not satisfy these conditions, the fitted model will not be able to accurately learn and reconstruct it.

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Title: Large Eddy Simulation of Momentum and Heat Transport in Urban Canopies: Computational Challenges and Gained Insights

Author(s): Elie Bou-Zeid, Qi Li, *Princeton U.*; William Anderson, *UT Dallas*; Sue Grimmond, *U. Reading*.

The transport of momentum and scalars, such as temperature, over complex rough surfaces modulates important systems in geophysics (such as cities and their microclimates) and engineering (such pin fin heat exchangers). Over such very rough surfaces, the transports of momentum and scalars are coupled but dissimilar - form drag controls momentum exchanges with the surface, while viscous processes continue to dominate for scalars. These differences give rise to distinct challenges for the accurate representation of flow and scalar transport, particularly at high Reynolds numbers, that should be simultaneously addressed. In this study, large-eddy simulations (LES) using the immersed boundary method are conducted for the problem. We discuss a new simple approach for the treatment of the Gibbs phenomenon that arises in the pseudo-spectral code, and then address wall-modeling challenges for high-Re LES of this problem. Validation against field (buildings) and laboratory (cubes) data is performed, and some initial insights on the turbulent transport mechanisms in and above the roughness sublayer are presented.

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Title: Monitoring of Temperature in Welded Plates With Monte Carlo Methods

Author(s): El Hadi Bouguerra, *Blida I U.*.

The use of the stochastic methods and in particular the Monte Carlo method for the resolution of the partial differential equations (PDE) was the subject of several researches by the past and particularly the conduction equation by Hadj-Sheikh. The main originality of those methods which consists to estimate the temperature in a particular point within the domain as the resultant of random walks from the border is that the temperature in a given point can be seen as the weighted contribution of each border. Moreover, since the random walks are equi-probable and independents, this lead to an interesting application to the monitoring problems. The temperature in a given point (to be watch) can be calculated once and the contribution of each border as weighted terms is determined. If there is a change on the border conditions, the temperature of the watched point can be immediately recalculated by a simple algebraic relation while with other numerical deterministic methods, the calculations should be redone. An application was made for the case of the welding of two steel plates by TIG process. The monitoring of the temperature of some places is important for the knowledge of the heat affected zone (HAZ). The temperature of a given point to be watched was determined by Monte Carlo method and the coefficients of the weight of each border was stored. After a change in a border condition, the temperature of the point was recalculated by the algebraic relation using the weighted coefficients previously defined. The results were compared with a direct method using finite differences which required a recalculation and showed a very good concordance. This feature can have a great importance in monitoring where a fast answer to any change of exterior conditions is needed. Keywords – Monte Carlo Methods; Monitoring; HAZ A. Hadj-Sheikh, Monte Carlo Methods, in W.J. Minkowycz, E.M. Sparrow, G.E. Schneider, and R.H. Pleitcher (eds), Handbook of Numerical Heat Transfer, chap 16, pp 673-722, Wiley New York, 1988.

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Title: Cyclic Steady States of Electro-Mechanical Devices and the High-Order Immersed Boundary Discontinuous-Galerkin Method

Author(s): Gerd Brandstetter, Sanjay Govindjee, *UC Berkeley*.

We discuss a recently developed high-order immersed boundary discontinuous-Galerkin method for the simulation of electro-mechanical devices, and its application to a new method in order to solve for cyclic steady states of electro-mechanical structures excited at resonance. The immersed boundary method features a high-order immersed boundary representation in combination with a high-order interpolation to accurately solve for the electrical field on a fixed grid with embedded boundary conditions [Brandstetter, G., and Govindjee, S., ``A high-order immersed boundary discontinuous-Galerkin method for Poisson's equation with discontinuous coefficients and singular sources,'' International Journal for Numerical Methods in Engineering, 101, 847-869 (2015)]. The method has been demonstrated to accurately capture the Maxwell-traction around nonlinear boundary features such as curved boundaries, and in particular in the presence of singularities around reentrant corners. In this presentation we show the application of a staggered electro-mechanical implementation to a Newton-Krylov shooting scheme, that enables one to solve for cyclic steady states of motion by a direct solution as an alternative to an expensive time-stepping through the transient phase from given initial conditions. The examples include the excitation of an elastic beam structure by an electrical field at resonance, as well as the dynamic steady-contact of a resonant switch excited at the fundamental mode. The computational speed-up over transient time-stepping for the presented examples follows the power law S=0.05*N^(1.1), where N can vary from 100 to many orders of magnitude higher.

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Title: Experimental and Simulation Analysis of Single Particle Impacts in Aluminum-Copper Alloys

Author(s): Luke Brewer, *U. Alabama*; Joseph Hooper, *Naval Postgraduate School*.

This talk will describe experimental and simulation results probing the dynamics of single particle impacts of aluminum-copper alloys onto steel substrates. Cold gas dynamic spray deposition is now being used to provide corrosion protection and repair for metallic structural components. This processing technique accelerates metal powder particles through a de Laval nozzle to supersonic velocities. The particles (10-40μm in diameter) impact the substrate and each other with sufficient kinetic energy to bond and build up a coating. Typical particle velocities range from 300-1200m/s, resulting in strain-rates on the order of 107-109/second. The exact physical mechanisms for deformation and bonding during these impacts are still not well understood. We have deposited a series of aluminum, copper, and aluminum-copper binary alloy, spherical particles onto highly polished steel substrates over a range of velocities and copper contents. We are using microscopic analysis techniques such as focused ion beam microscopy, electron backscatter diffraction, and precession electron diffraction to measure the extent of plastic deformation and the evolution in crystallite (grain) structure after impact. In parallel, we are using hydrocode simulations to model the transient stresses and dynamic loading in the sub-microsecond timeframe of the impact. Our simulations use the material point method (MPM) as implemented in the multiphase hydrocode Uintah. Standard material models such as a Mie-Gruneisen equation of state and Johnson-Cook viscoplastic/damage models are available for pure aluminum and copper, and our initial work has focused on validating that these models successfully reproduce experimental single-particle impact morphologies. We have also begun exploring the Preston-Tonks-Wallace model as a replacement for the more commonly used Johnson-Cook model. We have successfully sprayed single particles of pure aluminum and copper and have simulated their impact onto a steel substrate. The degree of particle flattening for pure aluminum upon impact was notable and somewhat surprising. The interface between the aluminum and steel appeared to be completely well bonded with no apparent deformation in the steel. In contrast, single copper particle impacts showed definite cratering into the steel substrate but less flattening than the aluminum. Simulations of the same impact events showed less severe deformation than observed in the experiment, but the lack of deformation on the steel substrate was similar. We also observed great sensitivity to the choice of constitutive model used for the simulation. The initial experimental results suggest that the true deformation of a single particle lies between the predictions of these two models.

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Title: Optimisation of Complex Flows with Discrete Sensitivity Analysis

Author(s): Oliver Browne, Gonzalo Rubio, Esteban Ferrer, Eusebio Valero, *U. Madrid*.

Sensitivity analysis measures the change in the output(s) of a mathematical system subject to a modification of the input(s). This analysis can be employed to determine the exact degrees of freedom of a system to modify to achieve a more stable and in most cases a more optimal state of the system. This could be applied any type of instability such as to suppress vortex shedding on an aircraft wing or provide acoustic control in an aircraft engine. A discrete framework for computing the global stability and sensitivity analysis to external perturbations for any set of partial differential equations was presented by Browne et al. [1]. This technique, that relies on adjoints, gives sensitivity fields which indicate where a forcing term or a base flow modification could help to stabilise the flow and provide a more stable solution. The aforementioned paper used flow past a circular cylinder at Re = 45 and flow past an open cavity at Re = 1400 to validate the methodology. Browne et al. also show that machine precision (near analytical) accuracy is achieved when computing the Jacobian with numerical differentiation by means of a complex-step approximation making the methodology very robust. The analysis in [1] was conducted on steady state stable base flows. This presentation will extend this methodology to consider steady state unstable base flows and geometry modifications using numerical continuation and discrete sensitivity analysis. [1] O. M. F. Browne, G. Rubio, E. Ferrer, and E. Valero. Sensitivity analysis to unsteady perturbations of complex flows: A discrete approach. International Journal for Numerical Methods in Fluids, 76, 12, 1088-1110, 2014

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Title: Parameterisation Estimation Using Data Assimilation

Author(s): Philip Browne, Matthew Lang, Peter Jan Van Leeuwen, *U. Reading*.

In the atmospheric sciences, some of the leading order terms of model error are known to come from unresolved subgridscale processes. These have long been recognised and the accepted practice has been to represent such subgridscale processes by so called parameterizations. These parameterizations are sometimes ad hoc, sometimes physically motivated. The choice of different parameterizations account for some of the major differences between different atmospheric models. In this presentation we shall introduce a rigorous data assimilation technique which can be used to estimate the model error in a dynamical model. The technique has the capability to estimate both the parameters used within parameterizations and the parameterizations themselves.

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Title: Numerical Approximation of PDEs Based on Compressed Sensing

Author(s): Simone Brugiapaglia, Stefano Micheletti, Simona Perotto, *Poly. Milano*; Fabio Nobile, *EPFL*.

We present a novel method for the numerical approximation of PDEs, motivated by the recent developments in sparse representation, and particularly by compressed sensing [3]. We name this approach CORSING (COmpRessed SolvING), and we introduced it in [2]. CORSING exploits the analogy between the measurements of a signal during the sampling process in compressed sensing and the evaluation of the bilinear form associated with the PDE against the test functions. In particular, we adopt a Petrov-Galerkin (PG) formulation of the PDE [1] and we aim at approximating the PG solution via a cheaper numerical method. The idea is to advantageously exploit the sparsity of the PG solution with respect to N suitable trial functions by evaluating the bilinear form against a randomized choice of m << N test functions. This yields an underdetermined m x N linear system, which is solved by means of a sparse optimization algorithm, e.g., a convex relaxation technique (Basis Pursuit), or a greedy algorithm (Orthogonal Matching Pursuit). A theoretical analysis of the CORSING procedure is presented, based on two new theoretical properties, i.e., the local a-coherence and the restricted inf-sup condition. Sufficient conditions on the parameters involved in CORSING guarantee the reliability of the method with arbitrarily high probability. Moreover, we provide error estimates depending on the best s-term approximation error in the trial space. Finally, a MATLAB implementation of CORSING confirms the robustness and reliability of the proposed strategy applied to advection-diffusion-reaction problems. [1] A.K. Aziz and I. Babuška. The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations, Academic Press, New York, 1972. [2] S. Brugiapaglia, S. Micheletti and S. Perotto. Compressed solving: a numerical approximation technique for PDEs based on compressed sensing. MOX-Report 43/2014, Politecnico di Milano, 2014. [3] D.L. Donoho. Compressed sensing. IEEE Trans. Inf. Theory, 52:1289-1306, 2006.

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Title: Interface Tracking For Modeling Thermal Decomposition of Polymer Foams

Author(s): Victor Brunini, Ryan Keedy, Sarah Scott, David Noble, Amanda Dodd, *Sandia Nat'l. Lab.*.

Polymer foams are used to provide thermal, electrical, and mechanical insulation in a variety of engineered systems. When exposed to abnormal thermal environments (e.g. fires) polymers decompose, producing significant amounts of gas that can lead to the pressurization and breach of sealed systems. The decomposition process also dramatically alters the heat transport mechanisms present in the system. Understanding this decomposition process is essential for modeling pressurization and heat transfer to components within these systems. X-ray videos taken during experimental tests clearly show the development and progression of an interface between regions of virgin foam and void space filled with gaseous decomposition products. The presence of this interface, and its impact on heat transfer, has not been addressed in prior modeling efforts. In this work we demonstrate a new modeling approach using the conformal decomposition finite element method (CDFEM) to track the foam decomposition interface. Explicitly tracking the interface provides two main advantages that should improve the model. First, as the foam recedes, the radiative heat transfer pathways in the system change. This is captured in the model by using a view factor radiation method and updating the view factors dynamically as the interface moves. Second, it allows for improvement upon prior approaches that either neglected gas convection entirely, or treated the whole domain as a porous medium. Interface tracking enables modeling of the gas-filled void region behind the decomposition front using an acoustically compressible Navier-Stokes treatment that is more reflective of reality. The gas flow in the void region is coupled to porous media flow in the virgin foam. The addition of these new physics to the model is intended to improve its predictivity, in particular allowing it to capture the impact of system orientation on heat transfer and pressurization due to convective and radiative effects. In addition to defining a novel modeling approach to the foam decomposition problem, this work addresses some of the significant numerical challenges that have arisen in attempting to solve such a tightly coupled multiphysics problem with dynamic geometry. Initial simulation results are presented; validation against experimental data will be pursued as future work. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. This is document SAND2015-0964 A

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Title: Performance Improvements for High-Order Discontinuous Galerkin Solutions to the Shallow Water Equations

Author(s): Steven Brus, *U. Notre Dame*.

The shallow water equations (SWEs) commonly serve as the basis for ocean circulation models used to study tides, riverine flows, and hurricane storm surge. Many applications require highly-resolved, computationally expensive, numerical simulations to provide accurate forecast and hindcast information for disaster mitigation. Discontinuous Galerkin (DG) finite element methods have many well-known advantages for solving conservation laws such as the SWEs. Among the most important of these is their ability to accommodate high-order solution approximations which result in increased error convergence rates. This can be leveraged to obtain large efficiency gains over low-order methods, as lower resolution is required to achieve the same error level. However, there are several considerations that must be addressed in order to realize these improvements in real-world applications. Since the efficiency gains of high-order methods rely on using larger element sizes, linear approximations are no longer sufficient to resolve boundaries and bathymetric features. This talk focuses on overcoming these two difficulties which pertain to the use of high-order solutions in practice. First, the piecewise-linear representation of no-slip land boundaries introduces numerical artifacts that are not present in low-order simulations. We demonstrate that the use of curvilinear, super/iso-parametric elements is necessary to obtain convergent solutions, especially in channel flow situations. The second challenge is creating a high-order representation of the bathymetry that allows bathymetric features to be resolved with a polynomial approximation inside the element. This is accomplished by using an implicit moving least squares technique to obtain a functional bathymetry description that determines the elemental approximation. In addition, the talk will discuss how the local, explicit nature of DG methods can be exploited to improve cache utilization and loop vectorization, lower parallel communication volume, and increase the overlap between communication and computation in the implementation of the algorithm. Together, these advances allow coarser, high-order solutions to provide similar accuracy to high-resolution, low-order simulations while being more computationally efficient. This makes the use high-order solutions a viable step forward over today's current state-of-the-art ocean circulation models.

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Title: Linearization Effects in Goal-Oriented Error Estimates for Nonlinear Problems

Author(s): Corey Bryant, *UT Austin*; Serge Prudhomme, *E. Polymtl*.

In this work, we examine the application of goal-oriented error estimation techniques to nonlinear problems. In general, the higher-order terms in the representation of the error in the quantity of interest are ignored without strong evidence that these terms are negligible. First, we discuss the conditions that allow one to extend the classical theoretical results for linear problems to the nonlinear problems, including Céa's Lemma, the Aubin-Nitsche Lemma, and a priori convergence estimates. Next, we review the application of goal-oriented error estimation to Burger's equation in 1D and analyze the influence of the higher-order terms on the error estimator. We repeat the same exercise for a nonlinear diffusion example that demonstrates a case in which neglecting these terms leads to poor accuracy of the estimates. Finally, we explore the effect of the higher-order terms on adaptive mesh refinement for 2D incompressible flow past a cylinder; we compare the performance of the typical refinement indicators, which neglect the nonlinear contributions, the refinement indicators based on the nonlinear terms only, and the refinement indicators that combine the nonlinear terms with the standard indicators. A conclusion of the study is that, while one may construct problems for which the nonlinear terms are significant, a representative example for which a classical adaptive method, based on the residual term only, fails to produce convergence to the exact solution of the problem, has yet to be found. [1] C. M. Bryant. On goal-oriented error estimation and adaptivity for nonlinear systems with uncertain data and application to flow problems. PhD thesis, The University of Texas at Austin, Austin, TX. 2014. [2] J. T. Oden and S. Prudhomme. Estimation of Modeling Error in Computational Mechanics. J. Comput. Physics, 182:496--515, 2002. [3] R. Verfurth. A Posteriori Error Estimation Techniques for Finite Element Methods. Numerical Mathematics and Scientifc Computation. Oxford University Press, 2013.

13th U.S. National Congress on Computational Mechanics
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Title: Adaptively Refined Multi-Patch B-Splines with Enhanced Smoothness

Author(s): Florian Buchegger, Bert Jüttler, *Johannes Kepler U. Linz*; Angelos Mantzaflaris, *Austrian Academy of Sci.*.

A new framework suitable for Isogeometric Analysis (IgA) on multi-patch domains is presented this talk. Our construction is motivated by emerging requirements in isogeometric simulations. In particular, IgA spaces should allow for adaptive mesh refinement and they should guarantee the optimal smoothness of the discretized solution, even across interfaces of adjacent patches. We introduce multi-patch B-splines with enhanced smoothness (MPBES) over interfaces. The new basis is constructed by combining boundary basis functions of neighbouring patches. If continuous geometries are read in, a least squares projection is used to increase the smoothness. Tensor-product B-spline bases can be used, but if local refinement is needed, we can also employ (truncated) hierachical B-spline bases. The process of creating a basis for MPBES is done automatically and implemented in the C++ library G+Smo. The new geometries can easily be exported back as separate patches, which ensures the connection with existing CAD systems. The advantages of the new spline space will be demonstrated by numerical examples, which show potential applications of the new basis in Isogeometric Analysis.

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Title: A Mechanobiological Approach to Relate Neurodevelopmental Processes to Brain Morphology

Author(s): Silvia Budday, Paul Steinmann, *F.A. U. Erlangen-Nuremberg*; Ellen Kuhl, *Stanford U.*.

The brain is our most important but least understood organ. Evidence increasingly suggests that brain morphology closely correlates with brain function. Malformations originating from early stages of development can result in severe neurological disorders. Understanding the mechanisms by which the cortex develops and folds is a fundamental problem in neuroscience. Brain folding is a highly dynamic process driven by various events on the cellular level: Primary folds form during the third trimester of gestation before we are born, secondary and tertiary folds occur and disappear throughout lifetime indicated by the ever-changing outer appearance of our brain. Although recent progress in cell characterization has provided further insight into the cellular processes during brain development, the mechanisms that cause the folded surface morphology remain poorly understood; leading explanations are incomplete and contradictory. Using the nonlinear field theories of mechanics supplemented by the theory of finite growth, we establish a model for brain growth [1] and show why our brain surface bifurcates into increasingly complex morphologies: Moderate growth generates a regular pattern of sinusoidal wrinkles, further continuing growth induces secondary instabilities associated with advanced irregular wrinkling modes [2]. Our model provides a mechanistic understanding of growth-induced primary and secondary instabilities and reveals the effect of cortical thickness, stiffness, and growth on the evolving buckling pattern [3]. It gives an indication of how disruptions on the cellular level propagate across the scales towards structural malformations on the organ level. Malformations of cortical development are common causes of mental diseases such as epilepsy and developmental delay. The severity of cognitive abnormalities scales with the distinctiveness of the cortical dysplasia. Understanding the spatio-temporal interplay of neurodevelopment can enhance early diagnostics of neurodevelopmental disorders including microcephaly, megalencephaly, pachygyria, lissencephaly, and polymicrogyria. Ultimately this can facilitate treatment and prevention of mental disorders. [1] Budday S, Raybaud C, Kuhl E. A mechanical model predicts morphological abnormalities in the developing human brain. Sci Rep. 2014;4:5644. [2] Budday S, Kuhl E, Hutchinson JW. Period-doubling and period-tripling in growing bilayered systems. Phil Mag. doi:10.1080/14786435.2015.1014443. [3] Budday S, Steinmann P, Kuhl E. The role of mechanics during brain development. J Mech Phys Solids. 2014;72:75-92.

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Title: Mechanobiology of Live Allograft Bone Systems (LABS)

Author(s): Elisa Budyn, Patrick Tauc, Eric Deprez, *ENS Cachan*; Morad Bensidhoum, Herve Petite, *U. Paris Diderot*; Eric Schmidt, *U. Illinois-Chicago*.

With increasing life expectancy in the US and in Europe, bone pathologies related to massive bone loss occurring later in life carry $5-$10 billion financial burden on the healthcare system. Human Haversian cortical bone is a complex hierarchical heterogeneous tissue resulting from continuous remodeling. Microdamage are resorbed by osteoclasts cells before tubular lamellar structures called osteons are formed by osteoblast cells issued from mesenchymal stem cells (progenitor osteocytes) laying collagen fibrils mineralizing with hydroxyapatite crystals glued together with non-collagen proteins and proteoglycans. Trapped osteoblasts further differentiate into mechano-sensitive mature osteocytes sensing stimulation from microdamage. Osteocytes bear 40 to 60 cytoplasmic processes extending into canaliculi to create a syncytial network with the neighboring cells. Because osteocytes regulate healthy bone turnover, it is essential to quantify the relationship between in situ mechanical stimulation and the cell biological response to improve allograft bone treatments. Live Allograft Bone Systems (LABS) using bone tissues from a human donor and bone cells from a patient were built to study the osteocyte in situ mechanobiology. Micro mechanical tests were conducted on the femoral bone samples and hybrid experimental and numerical top-down investigations imaged the growth of controlled nascent sub-microscopic damage near live osteocytes. UV, fluorescent and confocal microscopies coupled to a hierarchical multi-level numerical simulations fed the multi-scale local constitutive fracture mechanisms assumptions that were validated through scale by scale identification after the balance of the energies between the global and local scales. The finite element discretisation of the bone tissue morphology was explicit and the Dirichlet boundary conditions were calculated by digital image correlation. The model evaluates the in situ stress field near the cells and quantified nascent diffuse damage within osteon lamellae appearing from yield values of close to HAP (hydroxyapatite) strength to two-fold the intitial values when mineralized collagen fibers bridged cracks, confirming the known brittle/ductile fracture behavior of bone The in situ mature osteocyte environment was sudied based on the cell 3D morphology. The osteocyte morphology was reconstructed from confocal microcorospy images that were demultiplied to account for the information of finite thickness planes that had been compressed into single images of the 3D parallel plane segmentation. The canaliculi were traced by tubular geodesics and the edges of the contours of the cell body were detected by contrast enhancement techniques. The in situ cell biological response to mechanical load in particular its cytosolic calcium circulation was tracked by adequate fluorochromes.

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Title: Growth and Incompatibility: Experimental Characterization on Expanded Porcine Skin

Author(s): Adrian Buganza-Tepole, Ellen Kuhl, *Stanford U.*; Chad A. Purnell, Arun K. Gosain, *Lurie Children's Hospital*; Michael Gart, .

It is a well-known fact that tissues in vivo are not stress free. Furthermore, upon extraordinary loading conditions, tissues grow and remodel to restore mechanical homeostasis1. Growth of soft tissues has been described mathematically within a continuum mechanics framework by splitting the deformation gradient into a growth and an elastic contribution. The incorporation of the growth tensor leads to an incompatible intermediate configuration2. However, despite the popularity of such description, the incompatibility of the grown configuration and the resulting residual stresses have not been extensively characterized in experiments. Here we show the kinematic characterization of a porcine experimental scheme of tissue expansion. Our experimental design uses multi-view stereo, allowing for a flexible expansion protocol that matches clinically relevant conditions. We tattoo four rectangular grids on the back of a young pig, which naturally suggests the use of isogeometric analysis to describe the kinematics of thin shells using B-spline patches3. We implant and inflate two expanders, one spherical and one crescent-shaped expander, and we inflate them to a total volume of 225cc by bi-weekly inflations over a period of three weeks. At the end of the expansion process we excise the expanded and control rectangular grids. We further subdivide each patch into smaller rectangular regions. This last subdivision step reveals how, as biological tissues grow, they develop residual stresses due to the incompatibility that arises from the evolution of a continuous growth field over time. Our experiment sheds new light on the mechanics of growing materials and the importance of residual stresses in living tissues. 1Rausch MK, Kuhl E. On the effect of prestrain and residual stress in thin biological membranes. Journal of the Mechanics and Physics of Solids, 2013, vol. 61, no 9, p. 1955-1969. 2Ambrosi D, et al. Perspectives on biological growth and remodeling. Journal of the Mechanics and Physics of Solids, 2011, vol. 59, no 4, p. 863-883. 3Buganza-Tepole A, et al. Characterization of living skin using multi-view stereo and isogeometric analysis. Acta biomaterialia, 2014, vol. 10, no 11, p. 4822-4831.

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Title: Adaptive Multi-Scale Extended Finite Element Method for Modeling Two- and Three-Dimensional Cracks

Author(s): Quoc-Tinh Bui, Sohichi Hirose, *Tokyo Inst. Tech.*.

We develop an adaptive multiscale extended finite element method (AmXFEM) for two and three dimensional crack problems. An adaptive scheme based on a posteriori error estimator via the recovery stress is applied to detect the elements that are then refined, the transition between the fine and coarse mesh scales is treated as multiscale analysis using variable-node elements. The mismatching problem of different mesh levels is then solved. The AmXFEM reflects the robustness of an effective numerical method as the fine-scale mesh is only tackled to where it is required, e.g., cracked area. We consider some numerical examples of 2D and 3D crack problems to show the accuracy of the AmXFEM. In the presentation, we start presenting a short overview of the existing approaches that have developed for modeling cracks. We then describe our new approach that we have developed for 2D and 3D crack problems, the adaptive multiscale extended finite element method (Am-XFEM). We will subsequently show the accuracy and the effectiveness of the proposed Am-XFEM in modeling discontinuous problems through several numerical examples of stationary cracks. Close the talk with some conclusions.

13th U.S. National Congress on Computational Mechanics
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Title: A Large-Scale Ensemble Transform Method for Bayesian Inverse Problems Governed by PDEs

Author(s): Aaron Myers, Kainan Wang, Tan Bui-Thanh, *UT Austin*.

We present an ensemble-based method for transforming prior samples to posterior ones. This method avoids Markov chain simulation and hence discarding expensive work when a sample is rejected. The idea is to cast the problem of finding posterior samples into a large-scale linear programming problems for which efficient and scalable solver can be developed. Large-scale numerical results will be presented to demonstrate the capability of the method.

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Title: An Approach to Big-Data in Large-Scale PDE-Constrained Bayesian Inverse Problems in High-Dimensional Parameter Spaces

Author(s): Aaron Myers, Ellen Le, Tan Bui-Thanh, *UT Austin*.

We develop innovative approaches to address the big data challenge in large-scale inverse problems and UQ governed by expensive PDEs. The idea is to randomize the data to reduce the data dimension. We shall show that though the method is rooted in a Monte Carlo method, but the convergence is much faster than the the standard rate of law of large numbers. Various numerical results will be presented to demonstrate the effectiveness of our approaches.

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Title: A Composite Structure Model for Arterial Walls and its Interaction with Blood Flow

Author(s): Martina Bukac, *U. Notre Dame*.

Arterial walls of major human arteries are composite materials consisting of three main layers: intima, media and adventitia, separated by thin elastic laminae. We model arterial walls using a composite structure model consisting of a thin elastic layer and a thick elastic layer. The thin layer represents the intima-media complex, and it is modeled as a linearly elastic membrane. The thick layer represents the adventitia, and its elastodynamics are described using the 3D equations of linear elasticity. The wall interacts with a pulsatile blood flow, described by the Navier-Stokes equations for an incompressible, viscous fluid. The system is coupled via the kinematic and dynamic coupling conditions. We investigate the effects of the composite structural model on blood flow under physiological conditions. Our results reveal a new physical property of fluid-structure interaction problems involving thin interfaces with mass: the inertia of the thin layer regularizes solutions to the full problem.

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Title: A Storm Surge Model for the Coastlines of Japan with a Detailed Representation of the Low-Lying Area in Tokyo

Author(s): Shintaro Bunya, Takahiro Oyama, Masahiro Futami, *Mitsubishi Rsch. Inst., Inc.*; Satoshi Iizuka, Kohin Hirano, *Nat'l. Rsch. Inst. Earth Sci. & Disaster Prevention*.

This presentation introduces a storm surge model for the coastlines of Japan. The main targets of this model are 1) to predict storm surge heights along the entire coastlines of Japan and 2) to assess flooding risk of a low-lying area in Tokyo. We adopted the ADCIRC model, which uses the finite element method and unstructured triangular grids. The choice of unstructured grids and the high parallel computation scalability of the ADCIRC model allowed us efficient representations of geography to be able to model the coastlines with a 250m resolution of the entire Japan and with a 50m resolution of the Tokyo Bay area. The model contains a low-lying area in Tokyo as a floodplain, and coastal and riverine levees with surveyed and planned crest heights. The model contains approximately 1.2 million grid points. We validate the developed model under several conditions. The capability of reproduction of astronomical tides are tested in a one-year-long simulation with tidal potential and open ocean elevation boundary forcings. The result shows fairly good agreements in terms of harmonic constants with exceptions of the stations that reside in the distinguished sea areas connected with narrow channels with outer seas. We also test the model in two storm surge events that occurred in 2014. The meteorological focings (winds and pressure) are provided from a meso-scale operational model provided by Japan Meteorological Agency with a one-hour interval. In the event in October Typhoon Phanfone produced surges of approximately 0.7m at Tokyo observation station. The model reproduces the surge and astronomical tides simultaneously with a fairly good agreement. The maximum computed height is 0.65m. Some high-frequency seemingly numerical oscillations are observed. In December, a well-developed atmospheric depression produced surges of approximately 1.5m to 1.8m at Nemuro station in the west of Hokkaido island. The model reproduces the surge with a fairly good agreement. The maximum computed height is 1.4m.

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Title: A Mesh Objective Algorithm for Modeling Mode-I Cracks Using Quadrilateral Finite Elements

Author(s): Damon Burnett, *Sandia Nat'l. Lab.*; Howard Schreyer, *U. New Mexico*.

A computationally efficient mesh objective algorithm for modeling mode-I cracks is developed and implemented within a standard finite element formulation. The algorithm applies the crack opening displacements across the standard nodal degrees of freedom that is consistent with the smeared crack approach formalism. The primary reasons why the conventional smeared crack approach has not been successful have been identified as follows: (i) misalignment of the stress field around the cracked element, (ii) accumulation of spurious shear resulting in stress locking, and (iii) incorrect prediction of the direction of crack propagation. Two new and distinct techniques are developed to preclude both spurious shear accumulation and misalignment of the stress field around the crack tip to provide mesh objective results. A computationally efficient crack tracking algorithm is utilized to provide the correct crack path. It is demonstrated that the algorithm predicts load deflection curves and crack paths that are insensitive to both mesh size and orientation when modeling failure at an angle through a finite element mesh. The methods developed are expected to be applicable in higher dimensions and for other element types.

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Title: Advances in High-Dimensional Computational Measure Theory for Inverse Problems

Author(s): Troy Butler, *U. Colorado-Denver*.

There exist many practical hurdles in the high-dimensional extension of current computational measure-theoretic algorithms for quantifying uncertainties in input parameters to physics-based models. The measure-theoretic framework for formulating the stochastic inverse problem to a physics-based model is summarized, and we present a new non-intrusive sample based approach for estimating non-parametric probability measures in arbitrary finite-dimensional parameter spaces. There are various sources of error in such an approach including stochastic errors arising from the use of finite sampling and deterministic errors resulting from the numerical approximations to solutions of computational models. An a prior/a posteriori error analysis provides computable lower and upper bounds in probability of arbitrary events. We also discuss recent advances in the determination of an optimal observation network from a proposed set of quantities of interest in order to reduce the computational cost of solving the associated inverse problem with specific emphasis on reducing the number of samples required to approximate events to a specified accuracy. Other practical methods and theoretical results will be discussed related to the definition and approximation of function spaces representing spatially heterogeneous input parameters in computational models. Numerical examples will illustrate the various aspects of the theory presented.

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Title: An Assessment of Efficiency of Computation of Material Properties

Author(s): Tahir Cagin, *Texas A&M U.*.

In this talk, we will review the methods of calculation of Response Functions and the dynamic/transport properties of materials using microscopic fluctuations and dynamic time correlation functions. These formulation are developed for equilibrium Molecular Dynamics and Monte Carlo simulations, are widely used and widely deemed quite time consuming. We will provide insight gained over the years on computing both response functions and the material transport coefficients through examples, and specifically address the convergence issues. Alternative microscopic methods for determination of response functions and transport properties were established based on direct-equilibrium and direct-nonequilibrium / steady state formulations. We will compare and contrast these approaches through example applications.

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Title: Hermite WENO Schemes with Strong Stability Preserving Multi-Step Temporal Discretization Methods for Conservation Laws

Author(s): Xiaofeng Cai, *Xiamen U. / U. Houston*; Jun Zhu, *Nanjing U.* ; Jianxian Qiu, *Xiamen U.*.

In this presentation, we will describe a class of high order multi-step temporal discretization procedure for finite volume HWENO (Hermite weighted essential non-oscillatory) methods to solve hyperbolic conservation laws based on the work by Shu {SIAM J. Scient. Stat. Comput, v9 (1988), pp.1073-1084}. The key feature of the multi-step temporal discretization procedure is with variable time step and strong stability preserving (SSP). The Multi-step temporal discretization methods can make full use of computed information by Hermite WENO spatial discretization by holding the former computational values. Extensive numerical experiments are presented to demonstrate that the finite volume Hermte WENO schemes with multi-step discretization can achieve high order accuracy and maintain non-oscillatory properties near discontinuous region of the solution.

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Title: High-Performance Phase-Field Modeling

Author(s): Philippe Vignal, Adel Sarmiento, Adriano Cortes, Lisandro Dalcin, Victor Calo, *KAUST*; Nathan Collier, *Oak Ridge Nat'l. Lab.*.

Many processes in engineering and sciences involve the evolution of interfaces. Among the mathematical frameworks developed to model these types of problems, the phase-field method has emerged as a possible solution. Phase-fields nonetheless lead to complex nonlinear, high-order partial differential equations, whose solution poses mathematical and computational challenges. Guaranteeing some of the physical properties of the equations has lead to the development of efficient algorithms and discretizations capable of recovering said properties by construction. This work builds-up on these ideas, and proposes novel discretization strategies that guarantee numerical energy dissipation for both conserved and non-conserved phase-field models. The temporal discretization is based on a novel method which relies on Taylor series and ensures strong energy stability. It is second-order accurate, and can also be rendered linear to speed-up the solution process [1]. The spatial discretization relies on Isogeometric Analysis, a finite element method that possesses the k-refinement technology and enables the generation of high-order, high-continuity basis functions. These basis functions are well suited to handle the high-order operators present in phase-field models. Two-dimensional and three dimensional results of the Allen-Cahn, Cahn-Hilliard, Swift-Hohenberg and phase-field crystal equation will be presented, which corroborate the theoretical findings, and illustrate the robustness of the method. Results related to more challenging examples, namely the Navier-Stokes Cahn-Hilliard and a diffusion-reaction Cahn-Hilliard system, will also be presented. The implementation was done in PetIGA and PetIGA-MF, high-performance Isogeometric Analysis frameworks [2, 3], designed to handle non-linear, time-dependent problems. REFERENCES [1] P. Vignal, L. Dalcin, D. L. Brown, and V. M. Calo. Linear, unconditionally energy-stable time-integrators for phase-field models. in preparation, 2015. [2] N. Collier, L. Dalcin, and V. M. Calo. PetIGA: High-performance isogeometric analysis. arxiv, (1305.4452), 2013. http://arxiv.org/abs/1305.4452. [3] A. Sarmiento, A. M. A. Cortes, D. Garcia, L. Dalcin, N. Collier, and V. M. Calo. PetIGA-MF: a multi-field high-performance implementation of divergence-conforming b-splines. in preparation, 2015.

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Title: The ROMES Method for Statistically Quantifying Reduced-Order-Model Error

Author(s): Kevin Carlberg, Martin Drohmann, *Sandia Nat'l. Lab.*.

Reduced-order models (ROMs) employ a projection process to reduce the state-space dimensionality of computational models. These surrogate models often lead to more significant computational gains than `model coarsening' approaches, and higher robustness than data fits. For ROMs, model-error analysis has been limited primarily to computing rigorous a posteriori error bounds. Especially for nonlinear problems, however, these error bounds are often highly ineffective, i.e., they overestimate the actual error by orders of magnitude. To obtain tighter bounds, the ROM must be equipped with complex machinery that both increases the computational burden and is intrusive to implement. Further, error bounds are not directly useful for uncertainty quantification (UQ) problems, where a statistical model of the error that is unbiased and has low variance is more useful. This talk will discuss the reduced-order model error surrogates (ROMES) technique [1] for statistically modeling errors introduced by ROMs. The method relies on the existence of `error indicators' (e.g., error bounds, residual norms, dual-weighted residuals) that are cheaply computable artifacts of the ROM simulation yet correlate with the true (generally unknown) error between the ROM and the original model. The technique employs Gaussian-process regression to construct a mapping from these indicators to a distribution over the true error. The variance of this distribution can be interpreted as the (epistemic) uncertainty introduced by the ROM. Numerical experiments show that the method leads to a near-optimal expected effectivity in modeling normed errors. Additionally, employing a ROMES model as a correction for the output error can improve prediction accuracy by an order of magnitude; this contrasts with existing `multifidelity correction' approaches, which often fail for reduced-order models and suffer from the curse of dimensionality. Finally, ROMES can be used to generate error bounds with `probabilistic rigor', i.e., an error bound that overestimates the error with a specified probability. Reference: [1] M. Drohmann and K. Carlberg. “The ROMES method for statistical modeling of reduced-order-model error,” SIAM Journal on Uncertainty Quantification, in press (2014).

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Title: Numerical Modeling of Raveling in Open Graded Friction Courses (OGFC)

Author(s): Laura Manrique, Silvia Caro, *U. Los Andes*; Edith Arambula, *Texas A&M U.*.

Open Graded Friction Courses (OGFC), also known as Porous Friction Courses (PFC), are asphalt mixtures with high air void (AV) contents (i.e., 18 to 25%). These high void values provide the material the property of being permeable and the capacity for reducing tire-pavement noise. Consequently, the use of these mixtures at the top surface of asphalt pavements has shown benefits in two main areas: 1) safety (reducing hydroplaning), and 2) environment (noise reduction). Despite their benefits, some disadvantages associated with the use of these mixtures include a relative short service life (i.e., durability) as compared to dense-graded hot-mix asphalt, reduced noise reduction benefits with time (i.e., functionality), and the difficulty associated with winter maintenance activities. In terms of durability, the most critical pathology of OGFCs is raveling, a phenomenon defined as the progressive detachment of surface aggregates. Several empirical works have determined that raveling is mainly associated with binder softening, binder aging, and/or insufficient binder content. Some of these findings have been corroborated through the development of simplified numerical models. This work aims to complement existing numerical works of raveling in OGFC through a new Finite Element (FE) model implemented in Abaqus®. The model was used to study the mechanical response of realistic OGFC mixtures under different load and environmental demands. The selected OGFC mixtures had different material combinations, and used different total AV and asphalt binder contents. In addition, the influence of water (i.e., moisture diffusion and pore pressure) was also considered in the analysis. Input data for the model, as well as relevant information for its calibration, was obtained from an extensive experimental program conducted as part of this work. Initial results confirm that raveling is a complex process, and that load characteristics, binder-aggregate adhesion properties, and volumetric features are crucial for the initiation and propagation of this degradation process.

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Title: Comparison of Output Error Estimation for Finite-Element Discretizations of Convection-Dominated Flows

Author(s): Hugh Carson, David Darmofal, *MIT* ; Steven Allmaras, Marshall Galbraith, *MIT*.

Previous work by the authors has demonstrated a high-order fully-automated output-error based mesh adaptation method suitable for solving the Reynolds-Averaged Navier-Stokes equations. The high-order of accuracy is achieved with a discontinuous Galerkin discretization. While the adaptation method has proven to provide significant reduction in computational cost relative to second-order methods, the authors are currently exploring alternate high-order finite element discretizations. Specifically, continuous, discontinuous and hybrid (HDG/EDG) finite element methods are compared. Accuracy of both discretization and error estimates are considered, the latter an important factor in the effectiveness of solution adaptation methods.

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Title: Topology Optimization of Cellular Materials with Improved Non-Linear Mechanical Properties

Author(s): Josephine Carstensen, Reza Lotfi, James Guest, *Johns Hopkins U.*.

In recent years manufacturing technologies have advanced and made it possible to design and fabricate cellular materials with complex but prescribed topologies. Cellular materials in this context refer to porous materials with a representative unit cell that is repeated in all directions. Topology optimization offers a means to leverage these new manufacturing capabilities though a systematic design framework. Topology optimization has previously been used for unit cell design of materials with elastic properties such as optimized Young's, bulk, or shear modulus, and for the design of auxetic materials. Herein, we look to extend these approaches to design materials with properties that are governed by nonlinear mechanics, such as energy absorption. One of the primary challenges in this setting is the lack of unit cell upscaling techniques for nonlinear behavior. In its absence, we turn instead to the assumption of finite periodicity. The proposed formulation considers both geometric and material nonlinearities, and uses existing sensitivity analysis schemes as the backbone of the design algorithm [1-2]. The Heaviside Projection Method controls the manufacturability [3] and the Method of Moving Asymptotes is used as the gradient-based optimizer. Several new topologies are presented, including materials optimized for energy absorption, and experimental results of actual fabricated samples are discussed. [1] K. Maute and S. Schwartz and E. Ramm, Adaptive topology optimization of elastoplastic structures, Structural Optimization 15 (2), 81-91, 1998. [2] T. Buhl, C. Pedersen and O. Sigmund, Stiffness design of geometrically nonlinear structures using topology optimization, Structural and Multidisciplinary Optimization 19 (2), 93-104, 2000. [3] J. Guest, J. H. Prévost, and T. Belytschko, Achieving minimum length scale in topology optimization using nodal design variables and projection functions, International Journal for Numerical Methods in Engineering 61 (2) 238-254, 2004.

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Title: DNS of Strongly Accelerating Thermal Turbulent Boundary Layer

Author(s): Luciano Castillo, Guillermo Araya, Fazle Hussain, *Texas Tech U.*.

DNS of spatially evolving thermal (passive scalar) turbulent boundary layers with strong favorable pressure gradient (FPG) is performed by using a multi-scale dynamic approach for generating realistic inflow turbulent information. Re-laminarization under strong FPG is important in industrial applications and in fundamental studies such as drag reduction, atmospheric stability and wake-wake interaction in wind farms. In spite the fact that turbulent boundary layers have been studied for more than 50 years, the thermal turbulent boundary layer is not well-understood, and such simulations are non-existent today. Surprisingly, the thermal fluctuation, $\theta{'}^{+}$, and Reynolds shear stress, $\overline{u'v'}^{+}$ exhibit a logarithmic behavior in the meso-layer region (e.g., $30 \le y^+ \le 300$). The thickness of the log-region increases in the flow direction and with the strength of the acceleration. Moreover the mean thermal profiles do not exhibit a log region even in a ZPG region, and the outer wake region vanishes as in the mean velocity profiles for FPG. As the flow is drastically modified due to the pressure gradient, the thermal field is also changed. In spite of this similar trend of the mean velocity and thermal profiles, the Reynolds Analogy fails, having a sharp decrease in S_{t}/C_{f}. Furthermore, the maximum of $\overline{u'^2}^{+}$ and $\overline{v'\theta'}^{+}$ remains frozen over the ZPG and FPG regions, and the wall-normal heat flux, $\overline{v'\theta'}^{+}$, is independent of the strength of the acceleration. The spanwise and wall-normal components of the Reynolds stresses as well as $\overline{u’v’}^{+}$ continue to decay in the x-direction from ZPG (where maxima are nearly constant) to FPG (where they decay rapidly). However, a surprising result is an increase in the θ'^+ and $\overline{u’\theta'}^{+}$ components which change from constant in ZPG to linear rise as the FPG increases. Such behavior is a direct result of the stretching of the structures which then increases the streamwise heat flux and the turbulent thermal production terms $\overline{u’_{i}\theta{'}}\frac{\partial{\theta}}{\partial{x_i}}$. Lastly, the hairpin structures in the FPG region are significantly weaker than in the ZPG.

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Title: Methods to Include HMA Heterogeneity at the Multi-Scale Level Using Probabilistic Principles and Simulation Techniques

Author(s): Daniel Castillo, Silvia Caro, *U. de los Andes*.

Some recent work performed by the GeoSI (Geomaterials and Infrastructure Systems) group at Universidad de los Andes (Bogotá, Colombia) has been focused on studying material variability in geotechnical structures. A main conclusion from these studies is that, in general, material heterogeneity impacts the mechanical performance of pavement structures and, therefore, they constitute an area of interest in pavement engineering. This work describes five different approaches to include material heterogeneity into the numerical analysis of asphalt layers in flexible pavement structures. The steps are progressive in terms of computational efficiency, and they change from the 'macro' to the 'micro' scale. The five approaches are briefly stated as follows: 1. At the macro-scale, a basic approach to incorporate variability consists on generating 'replicates' of a pavement structure, each one with a homogeneous asphalt layer (i.e. mechanical properties are constant within the layer). While the asphalt material is considered homogenous, every realization has unique mechanical properties, i.e. a randomly generated value. 2. In reality, however, material properties within an asphalt course are heterogeneous. This can be computationally accounted for by dividing the asphalt layer into sections, and by randomly assigning different mechanical properties to each section. Random fields, a branch of the general stochastic theory, can be used to create these random, spatially correlated values. 3. A basic micro-scale modeling approach would include coarse aggregate particles that are embedded in a homogenous phase (i.e., fine matrix). Material variability can be incorporated to the fine matrix using simulation techniques, in a similar way to the first approach. 4. Since variability in the fine matrix does exist within a single realization, random fields theory can be used to account for the spatial heterogeneity of this phase—in a similar way to the second approach. This technique still considers coarse aggregates as a separate phase. 5. Finally, the most realistic approach consists on producing completely random microstructures. These microstructures are composed of randomly generated aggregates and air voids. Thus, this approach includes the three constitutive phases of an asphalt mixture, and it controls the properties of each phase (e.g. aggregate gradation and morphological properties, air void size and distribution, etc.). The advantages and disadvantages associated with each approach are presented, as well as some results obtained from incorporating these techniques into Finite Element analysis. In these analyses, special emphasis is made on the consequences of including material variability on the mechanical reliability of asphalt materials.

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July 27-30, 2015, San Diego, California, USA

Title: Predicting the Temperature-Dependence of the Yield Stress in Tungsten using Atomistically-Informed Crystal Plasticity Simulations

Author(s): David Cereceda, Jaime Marian, *UCLA*; Martin Diehl, *MPIE*.

We present crystal plasticity (CP) calculations of the plastic response of tungsten (W) single crystals in uniaxial and biaxial tensile tests. Our model is parameterized using atomistic calculations only, with no adjustable parameters. The constitutive relation employed in the CP model is based on a mobility function for screw dislocations that includes a full characterization of kink-pair energetics as well as of non-Schmid effects. We validate the model against existing experimental data of tensile tests in single-crystal W, with excellent agreement between the simulations and the measured data. We then extend the model to more complex deformation conditions and study the effects of temperature and strain rate. We provide the yield surface for biaxial tensile loading for a number of orientations in the standard triangle.

13th U.S. National Congress on Computational Mechanics
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Title: On Micromechanics Associated with Crack Growth in Quasi-Brittle Materials

Author(s): Mohamed Chabaat, Mokhtar Touati, *U. Sci. & Tech. Houari Boumediene*.

Micromechanics associated with crack growth in quasi-brittle materials are considered. It is known since the discovery of advanced devices such as high resolution microscope that crack growth characteristics contain information on the material strength of fracture mechanisms. On the other hand, there are sufficient experimental data evidencing that in most cases a crack growth is surrounded by a severely Damage Zone (DZ) which often precedes the crack itself. During its propagation, the DZ is characterized by few degrees of freedom (elementary movements) such as translation, rotation, isotropic expansion and distortion. On the basis of a stress field distribution obtained by the use of a Semi-Empirical Approach (SEA), which relies on the Green's functions, these driving forces corresponding to the mentioned degrees of freedom are formulated within the framework of the plane problem of elastostatics. SEA is proposed for evaluating the stress field and the different energy release rates. This approach is based on the representation of displacement discontinuities by means of the Green's function theory [2, 3]. This latest is used in a purely theoretical context. Herein, we suggest a more realistic model (arbitrary orientations of discontinuities rather than rectilinear ones) for which the result can be obtained using the experimental data and thus avoiding the difficulties of analytical solutions. Keywords: Stress, crack, damage, driving forces, energy release rate, Green's function, semi-empirical method. References [1] M. T. K. Takemori, Polymers Engng. and Sci., Vol. 22 (1982) 937-645. [2] M. Chabaat, S. Djouder and M. Touati, Int. J. of Applied Mech. and Mat. Vol. 3-4(2005) 243-252. [3] A. Chudnovsky, A. Dolgopolsky and M. Kachanov, Int. J. Solids Struct., 23(1987)1-21. [4] B. Budiansky and J. R. Rice, ASME, J. Appl. Mech., 40 (1973) 201-203. [5] Yi-Hen Chen, Int. J. Solids and Structures, 38 (2001) 3193-3212.

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Title: Multi-Scale Modeling of Microstructure Dependent Fracture in UO2

Author(s): Pritam Chakraborty, Yongfeng Zhang, Michael Tonks, *Idaho Nat'l. Lab.*.

The UO2 fuel pellets undergo extensive microcracking and fragmentation during service, which strongly affects the pellet-cladding interactions, fission gas release and consequently nuclear reactor performance. Experimental studies reveal that the porosity, pore and grain size distributions in the underlying microstructure have a strong influence on the fracture mechanisms and properties of the UO2 fuels. During operation, the inhomogeneous evolution of these microstructural features causes significant spatial variation of fracture properties in the pellets and can alter the thermo-mechanical-physical behavior of the UO2 fuel pellets. Hence, for accurate prediction of nuclear fuel performance, the development of microstructure-driven fracture models of UO2 fuels is necessary. In the present work, a hierarchical multi-scale modeling approach is pursued to characterize the porosity, pore and grain size dependent intergranular fracture in UO2. A phase-field model [1] is utilized to perform microstructure scale fracture simulations in which varying porosities, grain and pore sizes are considered. The model parameters are calibrated from molecular dynamic simulations performed on different grain boundary structures [2]. The response of the representative volume elements of the phase-field based microstructure scale simulation is then fitted to an engineering scale smear crack model. Subsequently, the prediction of the microstructure dependent fracture properties is made with experiments. The engineering scale model is then used to investigate the nuclear pellet fracture and pellet-cladding interactions under varying conditions. References: [1] C. Miehe, F. Welschinger, M. Hofacker, “Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations”, International Journal for Numerical Methods in Engineering, 83 (2010) 1273-1311. [2] Y. Zhang, P.C. Millett, M.R. Tonks, X-M Bai, S. B. Biner, “Molecular dynamics simulations of intergranular fracture in UO2 with nine empirical interatomic potentials”, Journal of Nuclear Materials, 452 (2014) 296-303.

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Title: Large-Eddy Simulation of Oil Dispersion in the Ocean Mixed Layer

Author(s): Marcelo Chamecki, Bicheng Chen, *Penn State U.*; Di Yang, *U. Houston*; Charles Meneveau, *Johns Hopkins U.*.

In April 2010, the Deepwater Horizon accident and the ensuing Macondo Gulf of Mexico oil leak at 1.5 km depth that lasted until mid July focused attention on the unique challenges associated with underwater blowouts in the deep ocean. Deep-water blowouts generate plumes of oil droplets and gas bubbles that rise through, and interact with, various layers of the ocean. These interactions strongly affect the subsequent arrival of parts of the plume at the ocean surface. An important part of the process occurs towards the latter stages, when plumes reach the ocean mixed layer (OML), where plume-turbulence interactions determine rates of dilution and bio-degradation. The focus of this presentation is on detailed simulations of oil transport in the ocean mixed layer using large-eddy simulation (LES). In the current LES, the velocity and density fields are simulated using a hybrid pseudo-spectral and finite-difference scheme. The oil plume is described by an Eulerian concentration field and it is simulated using a bounded finite-volume scheme. Simulation results show that the complex flow field originated from the interaction of wind-stress forcing, Coriolis effects and Langmuir circulations induced by surface waves gives rise to a wide variety of patterns in surface oil plumes. In particular, the size of oil droplets determines which features of the flow field impact the oil plume the most, affecting levels of dilution and the mean transport direction. Many of the flow features that impact oil transport in the ocean mixed layer are currently not included in parameterizations employed by regional/global ocean models. Some advances in development of improved parameterizations will also be presented.

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Title: PGD Reduced Models for Real-Time Model Updating Using Modified CRE and Kalman Filtering

Author(s): Basile Marchand, Ludovic Chamoin, *ENS Cachan - LMT Cachan*; Christian Rey, *Safran Tech*.

The Dynamic Data Driven Application Systems concept has received an increasing interest during the last decade, in particular in the Computational Mechanics community. The main idea is to create a feedback loop between a real system and its numerical model, in order to: (i) control the system evolution using model predictions; (ii) update model parameters using data measured on the physical system. A potential application may be real-time identification and control of damage evolution in structures [1]. In this talk, we focus on the identification step and model updating procedure which requires solving an inverse problem, usually ill-posed. The approach we propose is based on a coupling between the (stochastic) Kalman filtering [2] and the (deterministic) modified Constitutive Relation Error (mCRE) tool [3]. On the one hand, Kalman filtering enables effective data assimilation and prediction of system evolution from incomplete information; On the other hand, mCRE is a robust and powerful tool for complex model identification; leaning on energy functionals as well as duality and convexity properties, it has the ability to identify model parameters from highly corrupted data [4]. In order to reach the “real-time” feature of the inverse method, mCRE is here associated with reduced order modelling based on Proper Generalized Decomposition [5]. The proposed data assimilation strategy is applied to several mechanical problems with real-time identification/updating of evolving boundary conditions, thermal source localizations, or material parameters REFERENCES [1] E. Prudencio, P. Bauman, D. Faghihi, K. Ravi-Chandar and J. Oden, “A computational framework for dynamic data driven material damage control, based on bayesian inference and model selection”, International Journal for Numerical Methods in Engineering (2014). [2] R. Kalman, “A new approach to linear filtering and prediction problems”, Journal of Basic Engineering, pp 35-45 (1960). [3] A. Deraemaeker and P. Ladevèze, “A constitutive relation error model-updating method in structural dynamics with uncertain measurements”, Inverse Problems in Engineering Mechanics, pp 273-283 (2003). [4] O. Allix, P. Feissel, H. Nguyen, “Identification strategy in the presence of corrupted measurements”, Engineering, Computations, pp 487-504 (2005). [5] F. Chinesta, R. Keunings and A. Leygue, “The Proper Generalized Decomposition for advanced Numerical Simulations”, Springer (2014).

13th U.S. National Congress on Computational Mechanics
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Title: Control of the Multi-Scale Finite Element Method Using a Posteriori Error Estimation and Adaptive Strategy

Author(s): Ludovic Chamoin, *LMT-Cachan & INRIA*; Frédéric Legoll, *NAVIER & INRIA*; Claude Le Bris, *CERMICS & INRIA*.

In the context of multiscale analysis, the Multiscale Finite Element Method (MsFEM) is a powerful tool [1,2]. It uses basis functions which encode details of the fine scale description, and performs in a two-stage procedure: (i) offline stage in which basis functions are computed; (ii) online stage in which a cheap Galerkin approximation problem is solved. However, as in other numerical methods, a crucial issue is to control the accuracy of the numerical solution. In this work, we develop an a posteriori error estimate, and associated adaptive procedure, for MsFEM computations. For that, the concept of Constitutive Relation Error (CRE) based on dual analysis [3] is extended to the multiscale framework. We thus show how CRE can be effectively used to assess various error sources, and drive a robust adaptive algorithm. Conforming and nonconforming variants of MsFEM are considered, and goal-oriented error estimation is also addressed using adjoint-based techniques [4]. [1] Y. Efendiev, T. Hou, Multiscale finite element methods: theory and applications, Springer, 2009. [2] C. Le Bris, F. Legoll, A. Lozinski, An MsFEM type approach for perforated domains, SIAM Multiscale Modeling & Simulation,12(3):1046-1077, 2014. [3] P. Ladevèze, J-P. Pelle, Mastering Calculations in Linear and Nonlinear Mechanics, Springer, 2004. [4] P. Ladevèze, L. Chamoin, Calculation of strict error bounds for finite element approximations of nonlinear pointwise quantities of interest, International Journal for Numerical Methods in Engineering, 84:1638-1664, 2010.

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Title: High-Order Discontinuous Galerkin Methods on Pyramidal Elements

Author(s): Jesse Chan, Tim Warburton, *Rice U.*.

High order time-explicit nodal discontinuous Galerkin (dG) methods have grown in popularity over the past decade for reasons both mathematical and computational in nature. Optimized Lagrange interpolation nodes and sharp trace inequalities with explicit constants allow for explicit expressions for optimal CFL and penalty constants. Finally, the computational structure of dG methods on simplices and hexahedra allows for efficient implementation on architectures such as GPUs. In this talk, we present extensions of these aspects of dG methods to high order pyramidal elements.

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Title: Computational Modeling of the Mechanics of Progression of Anterior Vaginal Prolapse (AVP)

Author(s): Arnab Chanda, Vinu Unnikrishnan, Samit Roy, *U. Alabama, Tuscaloosa*; Holly Richter, *U. Alabama, Birmingham*.

Anterior vaginal prolapse (AVP) is an abnormality of the female pelvic system, usually caused by weakening of the pelvic floor muscles and musculo-connective tissue, due to events such as child birth, menopause and morbid obesity. With the progressive “dropping” of the urinary bladder into the anterior vaginal wall, AVP causes vaginal pain, difficulty emptying the bladder and sexual dysfunction. AVP is the most common type of pelvic organ prolapse, leading to over 300,000 surgeries performed every year in the U.S only, with less that 50% success rate. A closer look reveals that the high failure rates of these surgeries can be attributed mainly to the lack of understanding among medical practitioners and surgeons on the mechanics of AVP. In the 21st century, computational modeling has been used to study the mechanics of various biomechanical systems (such as the heart, skeletal system etc), and pathophysiology of diseases. Computational modeling of the mechanics of AVP progression can provide useful information to the urogynecological surgeons to predict disease progression in patients and develop effective surgical measures. In our current research, a full scale Finite Element (FE) model of the female pelvic system comprising the pelvic organs such as the urinary bladder, vaginal canal and the uterus, with the connective tissue and muscles are developed by segmentation of Magnetic Resonance Images (MRI). Non-linear hyperelastic tissue material properties from the literature are adopted for the pelvic organs and simulations are carried out considering the bladder to be filled to its maximum capacity. The effect of the bladder overpressure on the mechanical strains on the anterior vaginal surface are estimated. The effect of the varying vaginal tissue properties during stages of prolapse on the mechanical strains will also be presented.

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Title: A Comparative Study on the Parallel Performance of Locally Conservative Mixed Finite-Element Formulations for Darcy Problems

Author(s): Justin Chang, Kalyana Nakshatrala, Lennart Johnsson, *U. Houston*.

The finite element method (FEM) is one of the most popular numerical techniques for simulating flow through porous media. However, a serious drawback to the standard FEM is its inability to ensure local mass conservation. This physical property is extremely important when flow is coupled with transport, which is the case with many technological applications in subsurface modeling. Moreover, such applications may be extremely large-scale and require the computational domain to consist of millions to billions of degrees-of-freedom. In order to achieve optimal parallel performance for these large-scale problems, it is important for computational scientists to understand the data structures necessary to discretize the mathematical models, the communication overhead associated in assembling the equations, the performance of parallel linear solvers for resulting systems of equations, and how the various FEM behave with respect to the state-of-the-art high performance computing systems. Herein, we examine four commonly employed locally conservative mixed formulations: (1) stabilized mixed discontinuous Galerkin, classical mixed Galerkin using (2) lowest order Raviart-Thomas space and (3) P2/P0 interpolation, and (3) least-squares finite element method using augmented lagrangian. Each of these methods have been thoroughly studied and used over the years, but as far as we know, no comprehensive comparative study in the context of high performance computing has ever been reported in the literature. Herein, our goal is to systematically study the computational efficiency of these various methods by solving a benchmark 3D problem based on Darcy equations. We highlight key performance issues like strong scaling, floating-point operations (FLOPs) efficiency, and cache hits/miss ratio. These performance metrics aim to guide computational scientists on how to achieve optimal parallel efficiency across various computing architectures. Popular scientific libraries such as Firedrake, ParMETIS, PAPI, and PETSc are implemented for finite element assembly, mesh partitioning, performance tuning, and linear algebra, respectively. Details concerning the computational algorithms, solvers, and computing resources used are presented.

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Title: A High-Order Arbitrary Lagrangian-Eulerian Finite-Volume Method for Hyperbolic Conservation Laws

Author(s): Marc Charest, Jozsef Bakosi, Thomas Canfield, Alex Long, Nathaniel Morgan, Jacob Waltz, John Wohlbier, *Los Alamos Nat'l. Lab.*.

Arbitrary Lagrangian-Eulerian (ALE) methods incorporate dynamic mesh motion in an attempt to combine the advantages of both Eulerian and Lagrangian kinematic descriptions. They are especially attractive for modelling compressible flows since their moving meshes are able to capture large distortions of the continuum without excessively smearing free surfaces or material/fluid interfaces. It is desirable to combine these ALE descriptions with high-order spatial and temporal discretizations because, for a given accuracy, high-order methods offer the potential to greatly reduce computational costs. However, the application of high-order methods to ALE is complicated by changing mesh geometry and certain stability requirements such as geometric conservation. In addition to these challenges, it is also difficult to obtain accurate high-order discretizations of conservation laws without any unphysical oscillations across discontinuities, especially on multi-dimensional unstructured meshes. One high-order method that was proven to be efficient and robust for static meshes is the central essentially non-oscillatory (CENO) finite-volume method. Here, the CENO approach was extended to an ALE formulation on moving tetrahedral meshes. The proposed unstructured method is vertex-based and uses a direct ALE approach that avoids the temporal splitting errors introduced by traditional ``Lagrange-plus-remap'' ALE methods. The new approach was applied to the conservation equations governing compressible flows and assessed in terms of accuracy and computational cost. For all problems considered, which included various idealized flows, CENO demonstrated excellent reliability and robustness. High-order accuracy was achieved in smooth regions and essentially non-oscillatory solutions were obtained near discontinuities. The high-order schemes were also more computationally efficient for high-accuracy solutions, i.e., they took less wall time to achieve a desired level of error than the lower-order schemes.

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Title: A Posteriori Analysis of Implicit-Explicit (IMEX) Methods

Author(s): Jehanzeb Chaudhry, *Florida State U.*; Donald Estep, Simon Tavener, *Colorado State U.*; Victor Ginting, *U. Wyoming*; John Shadid, *Sandia Nat'l. Lab.*.

Implicit-Explicit (IMEX) schemes are an important and widely used class of time integration methods for parabolic or hyperbolic partial differential equations. In this talk, we develop accurate a posteriori error estimates for a user-defined quantity of interest for two classes of multi-step IMEX schemes for advection-diffusion-reaction problems. We cast the IMEX schemes in a variational format and perform a posteriori analysis to compute error in a quantity of interest for such schemes. Numerical results are presented that demonstrate the accuracy of the estimates for a representative set of problems.

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Title: Computational Modeling of Piezoresistive Response in CNT-Polymer Nanocomposites Using Material Point Method

Author(s): Adarsh Chaurasia, Gary Seidel, *Virginia Tech*.

The current work is focused on developing a computational micromechanics model using the Material Point Method (MPM) to study the piezoresistive response in Carbon Nanotube (CNT)-Polymer nanocomposites subject to large deformations. MPM follows an Eulerian - Lagrangian formulation allowing for transport of material points which carry the physical attributes of the material over a background computational mesh composed of finite elements. This allows for large deformation of the material without issues like mesh entanglement or singular matrices which would be expected in conventional finite element methods for such problems. In CNT-Polymer nanocomposites, electron hopping or quantum tunneling at the nanoscale has been identified as a key mechanism behind the observed macroscale piezoresistivity. The formation and disruption of the electron hopping pathways are highly dependent on intertube distances and under deformations can result in microstructural rearrangements in terms of electrostatic properties leading to transitions in material symmetries and component magnitudes of the effective electrostatic properties. In the current work, a quasi-static electromechanical MPM formulation is developed which allows for a continuum description of the non-continuum electron hopping between the CNTs at the nanoscale leading to an effective piezoresistive response. The electromechanical MPM framework allows for geometric nonlinearities in the solution under large deformations. Thus, the nanocomposite representative domain is subjected to large deformations resulting in highly nonlinear effective piezoresistive strain tensor coefficients and associated gauge factors. In addition, comparison with finite element method is presented in order to verify the accuracy of the solution and to observe the similarities and differences in the solutions obtained for the coupled electromechanical problem. These comparisons are presented in terms of local errors in the solutions and in effective properties calculated using the averaged field variables. Additional details about the convergence characteristics will be discussed in terms of material point density, number of background elements and the type of background elements. It is anticipated that the results presented herein will be useful in formulating effective strategies to solve complex coupled electromechanical problems for composite materials using MPM. Moreover, the observations made herein will help in obtaining controllable macroscale effective piezoresistive properties under large deformations which is essential for accurate correlation of strain state to the observed macroscale response, and thus, can contribute to better nanocomposite piezoresistive sensor design and interpretation.

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Title: Isogeometric Local H-Refinement Strategy Based on Multigrids

Author(s): Alexandre Chemin, Thomas Elguedj, Anthony Gravouil, *U. Lyon*.

Many algorithms for calculation with automatic grid refinement exist and very efficients ones are based on the Full Multigrid with localization (FMG) scheme [1]. This iterative scheme uses multigrid resolution initialized with a solution calculated on a coarse grid. If a given level of accuracy is not satisfied, a finer grid is constructed and a multigrid resolution is applied recursively to the new set of grids. Such algorithms show better rates of convergence than classical iterative resolution methods such as Gauss-Seidel or preconditioned conjugate gradients. A big obstacle using this kind of scheme with Finite Element Analysis (FEA) is to deal with the refinement of non-straigth geometric boudaries. FEA implies an approximation of the geometry constructed with the CAD software. Therefore, the construction of a fine grid from a coarse one without data on the exact geometry is not possible [2]. The introduction of IsoGeometric Analysis (IGA) [3] allows the calculation of mechanical problems using an exact representation of geometric boundaries. The use of IGA with FMG allows to circumvent the need to go back to the CAD geometry to refine curved boundaries. Here, we propose an automatic grid refinement with controlled accuracy algorithm for 2D elastic problems in the static case using IGA with NURBS basis functions and based on FMG with localization algorithm. A preliminary calculation is done on the geometric mesh from the CAD software, a finer grid is constructed and the FMG resolution starts. The precision criterion used to initiate a refinement is based on the energy density error between two successive grids. Prolongation operators used for that kind of approach are the natural ones, resulting from the standard geometric refinement algorithms used in CAD. The algorithm is tested for several classical problems and shows very good rates of convergence. Such a method can also be seen as an algorithm with automatic local grid refinement for IGA with controlled accuracy, avoiding propagation of refinement due to the tensor product structure of NURBS. The advantage of this method compared to hierarchical B-splines or T-splines is that we are able to perform local refinement for IGA in a less intrusive way for software already using a Galerkin formulation with NURBS basis functions. [1] Venner, C. H., & Lubrecht, A. A. (2000). Multilevel methods in lubrication, Vol. 37. Elsevier Science. [2] Adams, M., & Taylor, R. L. (2000). Parallel multigrid solvers for 3D-unstructured large deformation elasticity and plasticity finite element problems. Finite elements in analysis and design, 36(3), 197-214. Elsevier. [3] Cottrell, J. A., Hughes, T. J., & Bazilevs, Y. (2009). Isogeometric analysis: toward integration of CAD and FEA. Wiley.

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Title: On Rightward Axial Rotation in Early Chick Embryonic Development

Author(s): Zi Chen, *Dartmouth College*.

During early development, the embryonic chick brain exhibits a combination of progressive ventral bending and rightward torsion. This torsional morphogenesis process, also termed axial rotation, is one of the earliest organ-level symmetry-breaking events in development. Previous studies suggest that bending is likely caused by differential growth, but the physical mechanism for torsion remains poorly understood. Because the heart almost always loops in the same direction that the brain twists, researchers have speculated that heart looping affects the direction of axial rotation. Nevertheless, direct evidence did not exist, nor was the mechanical origin of such torsion well understood. In this work, experimental perturbations show that the bending and twisting of the brain tube are coupled and that the vitelline membrane exerts external loads necessary for axial rotation to occur. In addition, the asymmetry of the looping heart induces the chirality of the twisted brain. A computational model is built to interpret these findings in which both the effects of cross-sectional aspect ratio and the ratio between cervical and thoracic flextures on torsion are examined. Our work clarifies the mechanical origins of axial rotation and the associated left-right asymmetry in development, recapitulating D'Arcy Thompson's view of biological form as "diagram of forces."

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Title: Crack Propagation in Fibrillar Collagen Nano-Composites: Role of Polymeric Interfaces with Sacrificial Bonds and Hidden Length

Author(s): Qianli Chen, Ahmed Elbanna, *U. Illinois, Urbana-Champaign*.

Sacrificial bonds and hidden length (SBHL) in structural molecules provide a mechanism for energy dissipation at the nanoscale. It is hypothesized that their presence leads to greater fracture toughness than what is observed in synthetic materials without such features. Here, we investigate this hypothesis using a finite element model of two mineralized collagen fibril detaching along a polymeric interface with SBHL systems. Rate-and-displacement constitutive equations are used to describe the mechanical properties of the polymeric system. The model quantifies how the interface toughness increases as a function of polymer density and number of sacrificial bonds. Other characteristics of the SBHL system, such as the length of hidden loops and the strength of the bonds, are found to influence the results. The model also gives insight into the variations in the mechanical behavior in response to physiological changes, such as the degree of mineralization of the collagen fibril and polymer density in the interfibrillar matrix. The model results provide constraints relevant for bio-mimetic material design and multiscale modeling of fracture in human bone.

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Title: Research on the Key Technologies of Vibroseis Vehicle Roll-Over Protection Structure Based on Computational Dynamics Simulation, and Its Robust and Proactive Anti-Rollover Control

Author(s): Zhen Chen, Zhiqiang Huang, Shuang Jing, Qin Li, *Southwest Petroleum U.*.

Due to its environmental friendly performance and high-quality signal stimulation ability, vibroseis has become the key technology and equipment in oil and gas exploration. However, the work zones of the geophysical prospecting are mainly focus on the areas with complex terrain and harsh environment, such as desert, Gobi, piedmont zone, and mountain area. Therefore, rollover accidents happen frequently in the process of vibroseis vehicle driving, the safety of human life and apparatus are seriously threatened due to the extreme weight of vibroseis and its huge impact to the ground. We carry out research on the key technologies of vibroseis vehicle roll-over protection structure (ROPS) based on computational dynamics simulation, and its robust and proactive anti-rollover control. The rigid-flexible coupling nonlinear multi-body dynamics model of articulated vibroseis vehicle is firstly built to achieve its active anti-rollover robust control in field. Aim for roll-over in worst field condition, we establish systematic and scientific evaluation index system of safety protection and performance for ROPS; Using the methods of computational finite element dynamic to simulate the rollover and impact progress. The cab and its ROPS are mainly adopted tetrahedral meshing. In the combination with rollover crash test, we develop the research of the change pattern for stress-strain■impact deformation■impact acceleration of the key components and energy distribution when rollover protection structure are in collision■then explore the relationship between its structure and safety performance, mastering the mechanism of formation■development and the deformation control of plastic hinge in the process of collision; We conduct the study on safety protection and performance for different ROPS and combine the multidisciplinary optimization of structural reliability sensitivity analysis to optimize structure. Finally, we design a new rollover protection structure, which have the ability of actively induced deformation, and the performance of good energy absorption■avoiding continuous rolling, greatly enhancing the security protection performance of vibroseis vehicle in field operations, improving the technology level of oil and gas exploration.

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Title: Peridynamic Modeling of Pitting Corrosion Damage

Author(s): Ziguang Chen, Guanfeng Zhang, Florin Bobaru, *U. Nebraska-Lincoln*.

Corrosion damage is an extremely widespread danger to the durability and safety of structures, and there is considerable interest in understanding this phenomenon. Pitting corrosion can lead to accelerated failure of structural components by perforation, or by acting as an initiation site for cracking. The study of pit growth is the main focus in the community of corrosion modeling. These models have successfully predicted the corrosion rate and some are even able to capture the roughening of the corrosion surface. However, since these models consider that the corrosion reaction only affects the evolution of the metal surface, they cannot capture the changes in the mechanical properties in the layer immediately below the solid/liquid interface. These changes, such as embrittlement induced by corrosion or stress-dependence of the diffusion processes in corrosion, are determining factors in explaining how Stress Corrosion Cracking is triggered and how it progresses in time. In this presentation we introduce a novel peridynamic model for the evolution of damage from pitting corrosion. We model the anodic reaction in corrosion processes (in which electroplating is negligible) as an effective diffusion process in the electrolyte/solid system combined with a phase change mechanism using peridynamics. This allows autonomous movement of the interface. To capture subsurface degradation due to corrosion, we introduce a corrosion damage model based on a stochastic relationship that connects the concentration in the metal to the damage of peridynamic mechanical-bonds that are superposed onto diffusion-bonds. We study convergence of this formulation for diffusion-controlled regime. The model leads to formation of a subsurface damage layer, seen in experiments. We validate results against experiments on pit growth rate and polarization data for pitting corrosion. We extend the 1D model to the 2D and 3D, and introduce a new coupled model in which in addition to the concentration-dependent damage we allow material phase change based on damage. This coupled model accounts for broken mechanical bonds that enhance corrosion rate. We predict the pit shape and damage profile in materials with microstructural heterogeneities, such as defects, interfaces, inclusions, and grain boundaries. Keywords: Corrosion damage; Peridynamics; Diffusion; Microstructural heterogeneity Reference: Z. G. Chen and F. Bobaru, Peridynamic modeling of pitting corrosion damage, JMPS, in review.

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Title: Non-Reflection Scheme for Atomistic-to-Continuum Coupling

Author(s): Chuin-Shan "David" Chen, Chung-Shuo Lee, Yan-Yu Chen, *Nat'l. Taiwan U.*.

A non-reflection scheme is essential for any atomistic-to-continuum coupling simulation involving wave transmission. The study of non-reflection scheme for a discrete lattice dated back to 1970s and has recently been systematically extended to obtain time history kernel functions for crystal lattices. However, the method is derived in the frequency domain based on the assumption of the periodically repeating crystal lattice thus limits its usage to simple geometric boundaries, e.g., the planar boundary. In other words, typical corners in a MD simulation box cannot be handled through the procedure. In this talk, we will present a generalized real-space non-reflection scheme for atomistic-to-continuum coupling simulation. The time history kernel functions are derived in the real space instead of in the frequency domain. The assumption of periodically repeating crystal lattice adopted in the frequency domain is thus relaxed. The time history kernel functions for different crystal lattices are derived to demonstrate generality of the proposed method. The proposed scheme is implemented in LAMMPS and a reflection index is developed to monitor accuracy of atomistic-to-continuum coupling simulation.

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Title: Damping and Stiffening Forces of a Squeeze-Film Between Two Plates

Author(s): Shangyi Chen, *U. Missouri-Columbia*; Z.C. Feng, *U. Missouri-Columbia* .

This paper presents the analysis of the squeezed film damping and stiffening effect on the microstructure. The finite difference method for rectangular geometries is applied to solve the nonlinear isothermal Reynold's equation for the squeezed film [1]. The approach is validated by comparison to numerical and theoretical results for small squeeze numbers [2]. Most of existing research focus on the damping effect of the squeezed film. Our goal, however, is to quantify the stiffening effect, which affects the resonance frequency of the squeezed film and oscillator system. Attention is drawn to the elasticity of the air and the stiffening effect actually appears as a negative mass. The damping effect obtained from numerical solutions matches perfectly with the equivalent damping formula derived from the analytical formula. The dynamic response of sinusoidally forced oscillator involving one squeezed film is investigated by solving dynamic equation numerically in order to demonstrate the stiffening effect of the squeezed film. Three main parameters are considered: the initial gap of the squeezed film, the excitation amplitude, and the excitation frequency. The relationship between the amplitude of the steady-state sinusoidal response and the excitation frequency is determined. We obtain the dependence of the resonance frequency on the initial gap and the forcing amplitude and identify conditions when the stiffening effect must be included in dynamic study of the structures with squeezed films. References [1] Y-J. Yang and S.D. Senturia, Numerical simulation of compressible squeezed-film damping. Solid-State Sensor and Actuator Workshop, Hilton Head, South Carolina, June 2-6, 1996, 76-79. [2] M.H. Sadd and A.K. Stiffer, Squeeze film dampers: amplitude effects at low squeeze numbers. J. Eng. Ind. Trans. ASME, Ser. B 97 (1975), 1366-1370.

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Title: Advances in Particle-in-Cell Time Integration Techniques of Vlasov-Maxwell Equations for Collisionless Kinetic Plasma Simulations

Author(s): Guangye Chen, Luis Chacon, *LANL*.

The Vlasov-Maxwell equations describe first-principle kinetic plasma behavior in the collisionless regime. Although the Vlasov equation and Maxwell equations are linear when considered seperately, the coupling between the two is nonlinear, and feature a disparate range of temporal and spatial scales. Solving this set of equations efficiently and accurately has been (and still is) a tremendous challenge for computational physicists. The Particle-in-cell (PIC) method is a hybrid Lagrangian-Eulerian technique that employs the method of characteristic (using particles) for the Vlasov equation, combined with time-domain finite-difference method (on a grid) for Maxwell equations. The traditional PIC time integration method (e.g. leapfrog) is explicit, featuring both stringent temporal and spatial stability constraints [1]. Semi-implicit methods, introduced in the 1980s, cannot handle disparate particle and field time scales without significant loss of accuracy [1]. Modern multiscale particle-in-cell methods treat the equations in an IM/EX fashion: The field evolution is slow, and therefore an implicit large time step is employed; while the particles move fast, and a small timestep is employed for their orbits. The tight coupling of these two is enforced via nonlinear elimination, and makes use of particle sub-cycling and orbit-averaging. A Jacobian-free Newton-Krylov method drives global nonlinear convergence of the particle-field system. Compared to traditional explicit algorithms, the resulting solver is free of numerical instabilities, is more accurate (featuring exact conservation properties and demonstrably second-order temporal accuracy), and is orders of magnitude faster. We demonstrate the accuracy and efficiency properties of the algorithm with various numerical experiments. [1] Birdsall, Charles K., and A. Bruce Langdon. Plasma physics via computer simulation. CRC Press, 2014. [2] Chen, Guangye, Luis Chacón, and Daniel C. Barnes. "An energy-and charge-conserving, implicit, electrostatic particle-in-cell algorithm." J. Comput. Phys. 230.18 (2011): 7018-7036. [3] G. Chen, and L. Chacon. "An energy-and charge-conserving, nonlinearly implicit, electromagnetic 1D-3V Vlasov–Darwin particle-in-cell algorithm." Comput. Phys. Commun. 185.10 (2014): 2391-2402.

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Title: Modeling Polycrystalline Materials via a Novel Nonlocal Lattice Particle Framework

Author(s): Hailong Chen, Yang Jiao, Yongming Liu, *Arizona State U.*.

A novel nonlocal lattice particle framework, the Volume-Compensated Particle Model (VCPM), was proposed to study the elastic, fracture and elasto-plastic behavior of polycrystalline materials. Both 2D and 3D are considered. In VCPM, the domain of interest is decomposed into particles which are located at lattice sites according to various packing format, e.g., triangular packing in 2D and face centered cubic packing in 3D. The VCPM particles are connected via linear springs and the interaction between a typical particle pair not only has contribution from the connecting spring itself, but also affected by all its neighbors. Different from the classical way of treating material anisotropy by transforming the material stiffness matrix, the proposed framework rotates the underlying topological lattice structure consistently with the material crystallographic orientation while keeping the material stiffness matrix intact. For 3D cubic polycrystalline materials, the topological lattice structure in VCPM is the same as the materials' underlying lattice structure. Since the proposed framework is bond based, fracture can be easily modelled by bond breakage. Given the bond breaking rule, no external crack propagation criteria are required, the crack initiation and propagation is the natural outcome of bond breakage. This is one of the most advantage of the proposed framework for fracture modeling over other numerical methods. Distinct from the bond based Peridynamics, there is no limitation on the materials' Poisson ratio in the proposed framework. The simulation results are compared with both analytical solutions and experimental observations in the open literature. Conclusions and discussions are drawn based on the current study.

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Title: Numerical Bifurcation Analysis on Geomaterial Models and Its Application to Coupled Hydro-Mechanical Problems

Author(s): Qiushi Chen, *Clemson U.*; Alejandro Mota, *Sandia Nat'l. Lab.*.

Summary: Efficient and robust numerical algorithms for the detection of material bifurcation are crucial for multiphysics problems involving material instability and failure, such as localization and liquefaction. In this work, numerical analysis of bifurcation in the context of fully coupled hydro-mechanical problems is presented, where the focus is on the efficiency and robustness of the algorithms. The mechanical state of the geomaterial under consideration is given in terms of its fourth-order tangent moduli. The detection of material bifurcation is then posed as an optimization problem, where the determinant of the acoustic tensor is minimized with respect to directions. Different parametrizations of the acoustic tensor are proposed and compared with respect to their numerical robustness and efficiency. A numerical exact method to compute derivatives, i.e., Forward Automatic Differentiation (FAD) is applied to compute both the consistent tangent moduli in the material model and the Jacobian matrix used in solving the optimization problem using iterative method such as the Newton's method. Principal contributions: This work proposes and compares novel parametrizations of bifurcation detection and adopts a numerical exact method to computer derivatives in bifurcation analysis. Focusing on fully coupled problems, the proposed work will significant improve the accuracy and efficiency of bifurcation detection.

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Title: A Non-Linear, Phase-Field Model of Lithium Dendritic Growth on the Anode of a Lithium Ion Battery

Author(s): Lei Chen, Long-Qing Chen, James Chen, *Penn State U.*.

Lithium (Li) dendrite formation compromises the reliability of Li-ion batteries, either because dendrite pieces lose electrical contractor growing dendrite penetrates the separator and leads to internal short-circuiting. In this paper, a nonlinear phase-field model, accounting for the Butler-Volmer electrochemical reaction kinetics, is developed to investigate the dendritic patterns during an electrodeposition process. Using lithium electrodeposition as an example, the proposed model is first verified by comparison with the Nernst equation in a 1D equilibrium system. The nonlinear electrochemical kinetics is also confirmed at non-equilibrium condition. The dendritic patterns are examined as a function of applied voltage and initial electrode surface morphology. A design map is proposed to tailor the electrode surface morphology and the applied voltage to avoid undesired dendritic patterns.

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Title: A Multi-Scale Particle Method with Concurrent MD, DPD and MPM

Author(s): Zhen Chen, *DUT/MU*.

A Multiscale Particle Method with Concurrent MD, DPD and MPM Zhen Chen,1, 2* Shan Jiang,3 Yu-Chen Su2, Yong Gan,4 and Thomas D. Sewell3 1Department of Engineering Mechanics, Dalian University of Technology, Dalian 116024, China 2Department of Civil and Environmental Engineering, University of Missouri Columbia, MO 65211, USA 3Department of Chemistry, University of Missouri, Columbia, MO 65211, USA 4School of Aeronautics and Astronautics, Zhejiang University, Zhejiang 310027, China *Email: chenzh@missouri.edu Abstract Recent studies of nano energetic composites have necessitated the development of an effective multiscale discretizaiton procedure for simulating the responses of discrete nano/meso/micro structures to extreme loading conditions. A particle-based simulation procedure is being developed with a concurrent link between the Dissipative Particle Dynamics (DPD) method and the Material Point Method (MPM), and a hierarchical bridge from Molecular Dynamics (MD) to DPD, in order to effectively discretize the multiphase interactions associated with multiscale failure evolution. The proposed procedure has been illustrated using simulations of the dynamic and impact responses of discrete metallic nano/meso/micro structures [Chen et al., 2012 and 2014]. It appears that the DPD forces can be effectively coarse-grained using the MPM background grid, and that the concurrent link between the MPM and DPD enables near-seamless integration of constitutive modeling at the continuum level with force-based modeling at the mesoparticle level. The recent research focus is on the development of concurrent discretization among MD, DPD and MPM in a single computational domain. Representative examples will be presented in the conference to demonstrate the recent research results. References Chen, Z., Han, Y., Jiang, S., Gan, Y., and Sewell, T.D., “A Multiscale Material Point Method for Impact Simulation,” Theoretical and Applied Mechanics Letters, Vol. 2, 051003, 2012. Chen, Z., Jiang, S., Gan, Y., Liu, H., and Sewell, T.D., “A Particle-Based Multiscale Simulation Procedure within the Material Point Method Framework,” Computational Particle Mechanics, Vol. 1, pp. 147-158, 2014.

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Title: A Stabilized Quasi-Linear Reproducing Kernel Particle Method for Modeling Material Damages Under Extreme Events

Author(s): J. S. Chen, Edouard Yreux, Mike Hillman, *UCSD*.

Materials under extreme events, such as high-velocity impact and penetration processes, often lead to severe material fragmentation due to strong shock dynamics. Reproducing Kernel Particle Method (RKPM) relies on polynomial reproducing conditions to yield desired accuracy and convergence properties, but requires sufficient kernel support coverage of neighboring particles. Failure to meet this requirement leads to singularity in the moment matrix when basis functions with polynomial degree higher than zero are introduced. Further, low order quadrature such as nodal integration consumes much less CPU, but can yield non-convergent, unstable solutions. In this work, RKPM with quasi-linear approximation is first proposed to achieve nearly linear completeness in the approximation while avoiding moment matrix singularity that often occurs in events with material fragmentation. A stabilization scheme for nodal integration is further introduced based on Taylor expansion. It is shown that using this method, coercivity of the numerical solution can be increased with a dramatic decrease in cost compared to other common stabilization schemes. As such, enhanced accuracy and stability in the RKPM modeling of solids subjected to extreme loads and deformations such as penetration and blast events is achieved.

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Title: Dynamic Fracture in Functionally Graded Materials: A Peridynamic Model and Comparisons with Experimental Results

Author(s): Zhangqi Cheng, *Zhengzhou U.*; Yenan Wang, Guanfeng Zhang, Florin Bobaru, *U. Nebraska-Lincoln*.

Fracture in heterogeneous materials depends on their particular microstructure. Some functionally graded materials with inclusions that do not vary in size or shape among them have been analyzed experimentally in [1], and using a cohesive-zone finite element for the incipient stage of crack propagation in [2]. In this presentation, we discuss a comprehensive study for the dynamic fracture behavior of a glass-spheres-reinforced epoxy functionally graded material (FGM) with a bond-based functionally graded peridynamic model ([3]). We show results of convergence studies under uniform grid refinement (for a fixed size of the nonlocal region) and under decreasing the peridynamic horizon (for a fixed ratio of horizon size to grid spacing). We verify the model on elastic wave propagation in FGMs and compare computational results with analytical results based on the classical model. We then analyze dynamic fracture in a functionally graded plate with monotonically varying volume fraction of reinforcement under mixed-mode loading by eccentric impact relative to a pre-crack. We observe the strong influence boundary conditions and loadings have on the crack propagation behavior in terms of shape of crack path and crack propagation speed. This helps us understand the factors that control dynamic fracture in an FGM: material gradation, elastic waves induced by the impact loading, and the duration and magnitude of impact loading. Numerical results from the peridynamic model show that, in an FGM, reflected stress waves from the boundaries have less of an influence on crack growth than in a homogeneous and isotropic material. This is likely due to wave dispersion that takes place in FGMs, “dulling” the sharp wave fronts that may temporarily arrest a propagating crack in a homogeneous medium. The peridynamic simulation results for the crack path shape and crack propagation speed agree extremely well with experiments, through full failure of the sample. We conclude that in this type of FGM, with small same-shape inclusions relatively uniformly dispersed into the matrix, modeling of dynamic fracture is possible using a functionally graded peridynamic model that starts from a homogeneous representation of the material properties.

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Title: Two-Scale Design Optimization of Bending Plate and Beam Made of Material with Periodic Micro-Structure

Author(s): Gengdong Cheng, Liang xu, *Dalian U. Tech.*.

Two-scale design optimization of bending plate and beam made of material with periodic micro-structure Gengdong Cheng, Liang XU State Key Laboratory for Structural Analysis of Industrial equipment Department of Engineering Mechanics, Dalian University of Technology, 116024, Dalian, China The presentation briefly reviews the recent development of concurrent multi-scale structural and material topology optimization of 2D and 3D continuum based on asymptotic homogenization method and discusses its potential extension. Following the basic idea, this paper studies two-scale design optimization of thin bending plate and slender beam for a given amount of material. The plate macro-shape and boundary conditions are given. The plate is made of periodic homogeneous lattice or foam material. Both plate topology and lattice or foam material micro-structural topology are optimized concurrently. The design variables include artificial material density in both macro and micro-scale. The equivalent bending rigidity of the plate structure is obtained by the new implementation of asymptotic homogenization method, which is developed by Cheng et al.[1] and Cai et al.[2]. With this new implementation, the sensitivity of effective stiffness of bending plate with respect to the topological design variables in both macro-scale and micro-scale is obtained analytically and enables the application of gradient-based search algorithm in the optimization, which is one of the important advantages of asymptotic homogenization method. Various objectives and constraints are considered. Several numerical examples are given to show the potential of the proposed method. The method and algorithm is extended to two-scale design optimization of slender beam made of material with periodic micro-structure in its axis direction. Since there is no periodicity in its thickness direction, the size effect in the beam thickness direction is discussed. [1] G. D. Cheng, Y. W. Cai, L. Xu, Novel implementation of homogenization method to predict effective properties of periodic materials, Acta Mechanica Sinaica, 29 (4), 550-556, 2013 [2] Y. W. Cai, L. Xu, G. D. Cheng, Novel numerical implementation of asymptotic homogenization method for periodic plate structures, International Journal of Solids and Structures, 51 (1), 284-292, 2014

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Title: Efficient Design of Additive Manufactured Cellular Structures by Integration of Micromechanics Modeling and Topology Optimization

Author(s): Lin Cheng, Pu Zhang, Emre Biyikli, Yiqi Yu, Jakub Toman, Markus Chmielus, Albert To, *U. Pittsburgh*; Jiaxi Bai, *U. Pittsburg*.

Cellular structures are promising candidates to design lightweight, complex additive manufactured (AM) parts for reducing material cost and enhancing sustainability. In order to expedite the simulation-based design process of AM cellular structured parts, a new design-optimization methodology is employed, which takes advantage of both micromechanics modeling and topology optimization. First, the cellular structures are modeled using a computational homogenization approach based on micromechanics theory to obtain scaling laws that describe how the elastic constants vary with the relative density of a given cellular structure. Second, a topology optimization algorithm is developed to optimize a given 3D component within the framework of continuum topology optimization by using the homogenized cellular structure models. Both the minimum compliance problem and constrained stress optimization are studied and incorporated in the topology optimization toolbox. Third, a reconstruction algorithm is proposed to convert the relative density profile from topology optimization into explicit cellular structures in order to finish the cellular part design. The whole design-optimization process is implemented and validated by designing a cellular structured pillow bracket and conducting validation experiment on the resulting AM part.

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Title: A Void-Mechanics Modeling Procedure for the Mechanical Response of Additive Manufactured Materials

Author(s): Puikei Cheng, Jacob Smith, Sarah Wolff, Jian Cae, Wing Kam Liu, *Northwestern U.*.

Additive manufacturing (AM) has gained traction in recent years as a powerful and versatile tool for the fabrication of customizable parts, with metal-based AM being of particular interest for structural components. In broadening their applications and improving reliability, there is a need for better characterization of additively manufactured metals and their mechanical behavior. Large deformations in ductile materials are known to generate porosity through void nucleation at inclusion interfaces, followed by void growth, void coalescence, and fracture. Hence, the evolution of void volume fraction is a good descriptor for the mechanical behavior of ductile materials. An accurate void mechanics-based damage law is especially important for modeling additively manufactured metals since they tend to contain more voids than traditionally manufactured metals depending on the process parameters. The Gurson-Tvergaard-Needlemen (GTN) model was expanded with a shear term modification and made compatible with an experimentally-informed nonuniform void volume fraction initialization. The altered GTN model was implemented over a material domain containing an inhomogenous distribution of voids, inclusions, and surrounding matrix as a global constitutive law. Combined with microstructural data taken from SEM imaging of an AM component, this modeling procedure was able to simulate and reproduce experimental testing results. The void-mechanics modeling approach is therefore a promising direction for furthering the understanding of additively manufactured metals.

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Title: The Generation Of Random Correlated Tensor Fields

Author(s): Aaron Chesir, *MITRE Corp.*; Luis Costa, *U.S. Army ARDEC*.

Given the non-uniform nature of real materials at small scales (e.g. defects or voids in the crystal lattice), it seems necessary to model the constitutive relationships of real materials at those small scales to accurately model the behavior of the macro-scale object. However, it is impractical to characterize every detail of every point in that material. The only option, it seems, is to implement an averaging, or homogenization, to the model of the constitutive relation tensors. However, once the homogenization is performed, spatial statistical correlation begins to become apparent: The constitutive relations show that the thermodynamic state (e.g. stress) at one point is highly dependent on the thermodynamic state in a nearby region of the material. Experimentation can suggest likely distances of the effective correlation. One can now model the material using constitutive relations that although somewhat random from point to point, are highly correlated within a deterministic distance of each point. Multiple realizations of the constitutive relation tensor field serves the need for high-confidence models to predict material behavior in response to specified impacts upon the material. A method is presented by which multiple realizations of such tensor fields can be generated. The method has been implemented on a multi-processor-core supercomputer, and has been shown to be able to generate, in under 24 hours, a 60-million point, 2nd-order tensor field with the correlations specified as an arbitrary mix of an extensible library of primary correlation functions. As presented, a survey of prior efforts to generate Correlated Fields reveals many successful schemes that can each generate a single 2-dimensional field of scalar values with a variety of fixed spatial correlations. However, the survey suggests no success in the generation of multiple realizations of an arbitrarily-correlated point-tensor field such that the vectors of component realization values bear user-specified correlations, even when the field were restricted to only 1 dimension. The mathematical basis of the presented method is given. The architecture by which the presented method has been implemented on a supercomputer is described. Performance results are presented. The presentation concludes with a discussion of the limits of the current implementation, and approaches that can be taken to extend the flexibility of the inter-tensor-component correlation function specifications.

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Title: Polygonal Elements for Finite Elasticity

Author(s): Heng Chi, Glaucio Paulino, *Georgia Inst. Tech.*; Cameron Talischi, *Mckinsey*; Oscar Lopez-Pamies, *U. Illinois, Urbana-Champaign*.

Nonlinear elastic materials are of great engineering interest, but challenging to model with standard finite elements. The challenges arise because nonlinear elastic materials are characterized by non-convex stored-energy functions as a result of their ability to undergo large reversible deformations, are incompressible or nearly incompressible, and often times possess complex microstructures. In this presentation, polygonal discretization is introduced to study finite elasticity problems in two dimensions. We present both displacement-based and mixed polygonal finite elements, the latter of which consists of approximations of the displacement field and a pressure field, and discuss the issue related to their numerical integration. Moreover, the performance of the polygonal elements on convergence, accuracy and numerical stability is numerically studied. For demonstration purposes, we present the application of polygonal elements to two challenging problems of practical interest: i) the homogenization of filled elastomers with interphases and ii) the detection of cavitation instabilities in rubber.

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Title: Isogeometric Mesh-Free Analysis

Author(s): Sheng-Wei Chi, Shih-Po Lin, *U. Illinois, Chicago*.

Since the introduction of Element-Free Galerkin Methods by Belytschko et al. [1], meshfree methods have gained immense popularity and achieved great success in scientific and engineering computing. Meshfree methods enjoy advantages of being point-based methods, thus highly flexible in discretization; nonetheless, they are hardly recognized as an isogeometric analysis (IGA) [2], which has been commonly associated with NURBS-based methods. In this work, we attempt to integrate the accuracy of geometric representations in IGA and flexibility and adaptivity in meshfree approximations. The idea of the proposed method is that only the boundary surface that is immediately available from CAD tools is used to describe the exact boundary of the problem domain, and then meshfree particles are inserted inside the boundary surface, in a fairly flexible manner, for construction of the approximation function for analysis. Evidently, the proposed method features both exact geometry directly obtained from CAD and the flexibility in discretization. Nonetheless, numerical issues associated with meshfree approximation, such as the imposition of the essential boundary condition and the domain integration, need to be adequately treated to ensure the nice properties of meshfree approximation. We adopt domain integration schemes under the framework of Variationally Consistent Integration [3] and the Nitsche's method for imposing the essential boundary condition. Several benchmarks were tested to examine the effectiveness of the proposed method and numerical results were compared with those obtained by IGA. [1] Belytschko, T., Lu, Y.Y., and Gu, L., Element-Free Galerkin Methods. International Journal for Numerical Methods in Engineering, 1994. 37(2): p. 229-256. [2] Hughes, T.J.R., Cottrell, J.A., and Bazilevs, Y., Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Computer Methods in Applied Mechanics and Engineering, 2005. 194(39-41): p. 4135-4195. [3] Chen, J.S., Hillman, M., and Ruter, M., An arbitrary order variationally consistent integration for Galerkin meshfree methods. International Journal for Numerical Methods in Engineering, 2013. 95(5): p. 387-418.

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Title: The H-Version of the Method of Auxiliary Mapping for Higher Order Solutions of Crack Problems

Author(s): Maurizio Chiaramonte, Adrian Lew, *Stanford U.*; Yongxing Shen, *U. Michigan; Shanghai Jiao Tong U.* .

High order finite element solutions of crack an re-entrant corner problems in elasticity are noto- riously challenging to attain. The slow convergence rates for these classes of problems are tied to the low degree of regularity possessed by the solution. The need for high order solutions is motivated by long running simulations of crack propagation. In fact, as the error in the crack path grows non- linearly, it is of uttermost importance to accurately resolve the elasticity fields at each time step. The above ensures that the final computed crack paths are within reasonable tolerance of the exact one without excessive computational expenditures. To this extent, we develop higher order finite element methods for crack and re-entrant corner problems in elasticity. The method [2] exploits the a priori knowledge of the singular behavior of the fields to construct an alternate regular solution. Solving for the alternate problem yields optimal rates of convergence and high order of accuracy. Namely, standard finite element error estimates in the L2 and H1 norm are proved to hold, both for the alternate solution and the composed alternate solution. The salient feature of the method is the lack of additional degrees of freedom in comparison with standard Galerkin finite element formulation. Effectively, for the same computational cost we obtain a higher order of accuracy. Furthermore, unlike other state of the art tools, the method preserves the well conditioned nature of the system of equations and does not require the knowledge of the exact asymptotic behavior, hence the method can be readily applied to singular problems for which we are not endowed with an explicit asymptotic solution such as cracks in graded materials. The method is verified with respect several analytical solutions in two- and three-dimensions accounting for the possible curvilinear (non-planar) geometry of cracks as well as material inhomogeneities. Along with the above, we employ interaction integrals for curvilinear cracks [1] and the paradigm of Universal Meshes [3] for the simulation of crack evolution. Applications of the framework are showcased for complex fracturing problems. In particular, simulations of fracture instabilities in ther- moelastic materials subjected to large temperature gradients, where oscillatory fracture behavior is expected, will be used to demonstrate the robustness and capabilities of the presented tools. References [1] M. M. Chiaramonte, Y. Shen, L. M. Keer, and A. J. Lew. Computing stress intensity factors for curvilinear cracks. Int. Journal For Numerical Methods in Engineering, Submitted, 2015. [2] M.M. Chiaramonte, Y. Shen, and A. J. Lew. The h-version of the method of auxiliary mapping for higher order solutions of crack problems. preprint, 2014. [3] R. Rangarajan, M. M. Chiaramonte, M. J. Hunsweck, Y Shen, and A. J. Lew. Simulating curvilinear crack propagation with universal meshes. Int. Journal For Numerical Methods in Engineering, 2014.

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Title: Numerical Integration of Polynomials on Convex and Non-Convex Polygons and Polyhedra

Author(s): Eric Chin, N. Sukumar, *UC Davis*; Jean Lasserre, *U. Toulouse*.

We present a method that produces exact integration of positively homogeneous functions over convex and nonconvex polygons and polyhedra. On applying Stokes's theorem and using the property of homogeneous functions, we show that it suffices to integrate these functions on the boundary facets of the polytope. Furthermore, the method is recursively applied to reduce the integration of homogeneous polynomials over polygons and polyhedra to direct evaluation of related functions at only the vertices of the polytope. The results for homogeneous polynomials are generalized to the integration of arbitrary polynomial functions, which require the solution of a small system of linear equations. We provide illustrative examples in two and three dimensions that demonstrate the efficiency and accuracy of the method. The proposed integration scheme for polynomials can find applications in embedded and extended finite element methods, as well as conforming and nonconforming Galerkin methods, on polygons and polyhedra.

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Title: 4D Embryo-Specific Inverse Modeling of Blood Flow in the Chick Embryonic Heart Outflow Tract for Investigating Early Hemodynamic Changes Leading to Congenital Heart Disease

Author(s): Venkat Keshav Chivukula, Madeline Midgett, Sandra Rugonyi, *Oregon Health & Sci. U.*; Sevan Goenezen, *Texas A&M U.*.

Congenital heart diseases (CHD) or malformations in the heart at birth affect nearly 1% of newborns in the USA. Hemodynamics regulates cardiac morphogenesis by providing mechanical stimuli to cardiac cells. Altered blood flow introduced by surgical interventions in animal models has been shown to cause a variety of CHD; however the mechanisms by which altered hemodynamics in the embryonic heart lead to CHD are still unclear. The current study focuses on characterizing the hemodynamics in the chicken embryonic cardiac outflow tract (OFT) during the Hamburger and Hamilton(HH) developmental stage HH18 (corresponding to 28 days in the human embryo). At HH18 the heart is tubular and the OFT connects the embryonic ventricle to the arterial circulation, and was chosen for investigation as major congenital defects are known to originate from this region. Hemodynamic disruption was achieved by OFT banding in which a suture is tied around the OFT, thereby restricting motion and constricting lumen area. Structural images and blood flow velocities from the OFT were acquired using a custom Optical Coherence Tomography system. Embryo-specific 4D (3D + time) computational fluid dynamics (CFD) models were generated using a custom image segmentation algorithm. An inverse-method based optimization algorithm was used to replicate the embryo-specific hemodynamics for each embryo. Appropriate boundary conditions were estimated by optimizing velocities at a specific point within the lumen to within 1% of the experimentally measured velocities. CFD simulations were performed using ADINA for a representative model of normal and hemodynamically altered (OFT banded) embryo OFT over the complete cardiac cycle. OFT banding constricted the lumen area by 30%, resulting in doubling of peak velocities through the lumen at peak systole. The pressure drop for achieving the experimentally observed flow through the lumen was higher by 50% for the banded embryo compared to the normal embryo. The maximal wall shear stress (WSS) doubled for the banded embryo over the normal embryo at peak systole, with the WSS distribution over the OFT being highly heterogeneous for both embryos. This abnormal hemodynamic environment in the developing heart exposes the cardiac cells to altered levels of hemodynamic stimuli, consisting of both altered stretch and WSS which are known to trigger signalling pathways that interfere with normal cardiac development. The computational models developed by our research group are being used to characterize 4D blood flow and to examine the effect of altered hemodynamics on cardiogenesis.

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Title: Accurate Crack Path Representation in a Cohesive Surface Element Approach for Mixed-Mode Fracture Analysis

Author(s): Habeun Choi, Kyoungsoo Park, *Yonsei U.* .

A cohesive surface element approach is generally limited for a crack path representation because surface elements are inserted between element boundaries. In order to accurately represent a crack path for a mixed-mode fracture, an element splitting technique is proposed in conjunction with an extrinsic cohesive zone model. When the principle stress at a crack tip is greater than the cohesive strength, a continuum element is split and a cohesive surface element is adaptively inserted along the principle stress direction. Changes of local element connectivity are updated by utilizing a topology-based data structure (TopS)[1]. A potential-based cohesive model (PPR model) is employed for the constitutive relationship of the cohesive zone model[2]. Finally, mixed-mode fracture examples are illustrated in order to verify and validate a proposed computational framework. References [1] Celes, W., Paulino, G. H., & Espinha, R. (2005). A compact adjacency■based topological data structure for finite element mesh representation. International Journal for Numerical Methods in Engineering, 64(11), 1529-1556. [2] Park, K., Paulino, G. H., & Roesler, J. R. (2009). A unified potential-based cohesive model of mixed-mode fracture. Journal of the Mechanics and Physics of Solids, 57(6), 891-908.

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Title: Framework for Double Porosity Flow in the Finite Deformation Range

Author(s): Jinhyun Choo, Ronaldo Borja, *Stanford U.*.

Aggregated structures or fissures in geomaterials often form pores much larger than pores between particles. A key challenge in poromechanical modeling of these materials under large deformation is how to consider fluid flow through pore structures that collapse at two scales. To tackle this challenge, we develop a computational modeling framework for double porosity flow in the finite deformation range. Conservation laws for deformable double porosity media are reformulated to include finite deformation effects. To link solid deformation with porosities separately evolving at two scales, we propose a multiplicative decomposition of the deformation gradient with respect to pore scales. For the mechanical modeing we extend a finite strain Cam-clay model to incorporate aggregated structures, validating it against experimental results of an aggregated soil. Through numerical examples we demonstrate poromechanical processes involving flow through pore structures that heterogeneously collapse at two scales.

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Title: Development and Experimental Validation of a Dual-Core Self-Centering Sandwiched Buckling-Restrained Brace (SC-SBRB) Using High-Strength Steel Tendons as Tensioning Elements

Author(s): Chung-Che Chou, Wen-Jing Tsai, Ping-Ting Chung, *Nat'l. Taiwan U.*.

Buildings designed based on current earthquake-resisting frame systems provide life safety performance in a large earthquake, but have significant structural damage and residual drifts due to energy dissipation in some structural members. The damage may lead to difficult or expensive to repair buildings after an earthquake. Therefore, development of structural systems that can dissipate seismic energy, minimize structural damage, and return to their original position, or called self-centering, after an earthquake is needed. This paper presents a viable solution that was used to validate the kinematics and mechanisms of an innovative brace member by multiple cyclic tests. The new brace is called a dual-core self-centering sandwiched buckling-restrained brace (SC-SBRB), which combines the excellent energy dissipation of the sandwiched buckling-restrained brace (SBRB) with the self-centering property of the dual-core self-centering brace (DC-SCB). Chou et al. [1, 2] proposed a steel dual-core self-centering brace (DC-SCB), which utilizes three conventional steel bracing member sets and two sets of conventional tensioning elements that are in a parallel arrangement. Two inner cores and two sets of conventional tensioning elements in a brace member are used to double the axial elongation capacity of the brace. A SBRB that is composed of an energy dissipative core and a pair of buckling-restrained member sandwiched together by high-strength bolts provides stable energy dissipation [3]. The SC-SBRB is essentially a SBRB positioned alongside the DC-SCB and creates both self-centering and energy dissipation properties when it is loaded in either tension or compression. A 7860 mm-long SC-SBRB, which uses ASTM A572 Gr. 50 steel as bracing members and ASTM A416 Grade 270 steel tendons as tensioning elements, is tested six times to validate the kinematics of the brace and evaluate its cyclic performance. The test program demonstrated that the proposed SC-SBRB behaves as the mechanisms and provides stable hysteretic response with appreciable energy dissipation, self-centering ability, and large maximum deformation capacities before fracture of the steel core. (1) Chou C.C., Chen Y.C. (2015).Development of Steel Dual-Core Self-Centering Braces: Quasi-Static Cyclic Tests and Finite Element Analyses. Earthquake Spectra, 31(1), 247-272. (2) Chou C.C., Chung P.T. (2014).Development of Cross-Anchored Dual-Core Self-Centering Braces for Seismic Resistance. J. Constructional Steel Research, 101, 19-32. (3) Chou C.C., Chen S.Y. (2010).Subassemblage Tests and Finite Element Analyses of Sandwiched Buckling-restrained Braces. Engineering Structures, 32, 2108-2121.

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Title: Wind Energy Simulations in a Mesoscale-LES Nested Model Framework

Author(s): Fotini Chow, Nikola Marjanovic, *UC Berkeley*; Jeffrey Mirocha, *LLNL*; Branko Kosovic, *Nat'l. Center Atmospheric Rsch.*; Matthew Aitken, Julie Lundquist, *U. Colorado-Boulder*.

Accurate assessment of wind farm performance requires consideration of the interaction of wind turbine wakes. In a modeling environment, these wakes must be considered within the full context of weather events and how they are represented in the model, including effects of local topography, land use, and turbulence. To this end, we have implemented generalized actuator disk (GAD) and generalized actuator line (GAL) models to represent turbine wakes in the Weather Research and Forecasting (WRF) mesoscale atmospheric model. The GAD represents the effects of thrust and torque from a wind turbine on the atmosphere within a disk representing the rotor swept area, while the GAL tracks the location of individual turbine blades and applies the normal and tangential forces at the temporal location of each blade instead of distributing the total force of all the blades over the actuator disk. The forces applied by the blades on the atmosphere are parameterized using blade element theory and the aerodynamic properties of the blades. WRF is used here in a grid nested configuration starting from the mesoscale (~ 10 km resolution) and ending with fine scale resolutions (~1-10 m) suitable for large-eddy simulations (LES). At the finest scales we resolve the thrust and torque forces from the turbines using the GAD and GAL models. Both models include realistic representations of the turbine, including real-time yaw and pitch control to respond to changing flow conditions. We investigate both idealized and real model configurations at a wind farm to demonstrate the capabilities of the models. The main advantage of the GAL model is that it can represent the effect of tip vortices in the near wake region and therefore results in better overall prediction of wake deficits compared to the GAD model. In the far wake region, the differences in wake deficits are nearly indistinguishable. We also discuss issues related to turbine wake modeling at different model resolutions.

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Title: Bayesian Karhunen - Loeve Expansions: A Random Subspace Approach

Author(s): Kenny Chowdhary, *Sandia Nat'l. Lab.*.

Principle Component Analysis, or PCA for short, is a common statistical procedure for reducing the dimensionality of a given data set. In a nutshell, PCA allows one to represent a data set as a linear combination of uncorrelated random variables via a change of basis. Moreover, this transformation is optimal in the least squares sense. In the first part of this talk, we will briefly go over the basics of PCA through examples. Then we will introduce an alternative Bayesian inference approach to PCA in which the basis vectors themselves are random. This will allow us to quantify the uncertainty in the principle components when we have limited samples of the data. In order to perform the Bayesian inference, an efficient Gibbs sampler over the space of orthonormal matrices is utilized.

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Title: Toward Exascale-Era Parallel Mesh Generation

Author(s): Nikos Chrisochoides, Andrey Chernikov, Daming Feng, Christos Tsolakis, *CRTC Lab, Old Dominion U.*.

In this paper we will present a top down approach for guaranteed quality massively parallel mesh generation and its broader impact to real-time medical image computing. First, we will present a telescopic algorithmic approach to explore a billion-way concurrency by using a hierarchy of abstractions that leverage the memory and network hierarchy of current and emerging multi-layered parallel architectures. Then we will present our preliminary performance data from medical image computing.

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Title: Physics-Based Computational Modelling of Knitted Textile Architectures

Author(s): Daniel Christe, Chenyang Mo, Krzysztof Mazur, Aditi Ramadurgakar, Shane Esola, Antonios Kontsos, *Drexel U.*.

Knitted fabrics are hierarchically structured materials exhibiting a complex set of structure-property-behavior relations. Compared to other materials such as fiber-reinforced composites or metals, knitting gives the designer much finer control over the manufactured structure, fitting the broader “materials-by-design” framework. While manufacturing capability is sufficiently advanced to allow digital morphological design and production of elaborate knit structures from a diverse array of input materials, a lack of predictive simulation capability hinders progress in certification and deployment of smart garment devices, which are envisioned as tailorable material platforms for applications such as actuation or medical sensing. A key objective of this work is to develop robust data-driven simulation tools to study mechanical/multi-physics behavior of smart textiles. To this aim, we implement an integrated computational materials engineering (ICME) strategy linking multiscale mechanical testing, numerical simulation, computational mechanics, and manufacturing. Specifically, mechanical testing of selected yarn grid level pattern(s) in parallel with full-field strain mapping via digital image correlation was conducted as part of a broader hierarchical characterization scheme from single fiber to fabric levels. The internal structure was imaged in two and three dimensions using a combination of optical, scanning electron microscopy, and microcomputed X-ray tomography. Simulation-wise, geometric representation of knit structures was accomplished with with consideration of actual manufacturing process parameters. Computational mechanics methods were employed to investigate the role of structure and material properties in determining deformation behavior of knitted materials, with a goal to provide quantitative feedback to manufacturing.

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Title: Higher-Order Immersed B-Spline Finite Elements

Author(s): Matija Kecman, Fehmi Cirak, *U. Cambridge*.

We present novel integration procedures as an extension to our previous work on immersed finite element methods applied to problems of shape/topology optimisation [1] and fluid-structure interaction [2]. A key feature of our approach is the use of implicit geometry representations, which enables decoupling of analysis from geometry and provides the basis for our new integration procedures. The implicit geometry can be obtained directly or constructed from a wide variety of input data types by leveraging a rich theory developed by the computer graphics community. The construction step is frequently inexpensive, and in many cases (including some spline-based surfaces) purely algebraic and exact. Additional enhancements to conventional engineering workflows, such as robust handling of poor quality CAD input and filtering of small geometric details, which can be difficult to implement for methods based directly on parametric geometry, are almost automatic. Our proposed method recovers surface and volume integration domains defined by the implicit geometry using simple template-based tessellation procedures. First, we generate a linear reconstruction of the implicit geometry by marching over cut cells and selecting the best tessellation from a small number of candidates. Next, a higher-order tessellation is constructed by introducing additional nodes and placing them on the immersed geometry. The use of implicit geometry makes the intersection computations used in this step highly robust and simple to implement. The algorithm is further augmented with a facility to preserve sharp features and specially-designed refinement routines, which ensure cut-cell topology is restricted to a small set of possibilities. Although our method is implemented in an existing framework using b-splines defined on a Cartesian background grid, this is not a principle restriction and it can be applied to general unstructured background meshes. Furthermore the method does not require complicated data-structures and generates integration meshes local to each background cell, independent of all neighbours. The latter property is highly desirable in our case since integration meshes are automatically aligned with the knot-spans of the background splines thus side-stepping additional complexity present in other approaches. [1] K. Bandara, T. Ruberg and F. Cirak. Shape optimisation with multiresolution subdivision surfaces and immersed finite elements. Submitted for publication, 2014. [2] T. Ruberg and F. Cirak. A fixed-grid b-spline finite element technique for fluid-structure interaction. International Journal for Numerical Methods in Fluids, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: Designing with Topology Optimization

Author(s): Brett W. Clark, *Sandia Nat'l. Lab.*.

The combination of topology optimization and additive manufacturing enables a design space and paradigm that produces designs driven by functional requirements as opposed to designs constrained by manufacturing processes. Instead of analysis as an after-thought in validating existing designs, physics simulations drive the placement of material to define optimal designs. The adoption of topology optimization as a design tool is often hindered by the expertise required to use the technology. Furthermore, the cost of meaningful physics calculations for topology optimization on real world problems often requires significant horsepower only provided on large HPC platforms. At Sandia National Labs we are developing a design environment aimed at making topology optimization easy to use, based on powerful physics capabilities, and with the option to link directly to high performance computing platforms. This presentation will demonstrate our existing capabilities and describe our ongoing work toward a truly function-based design environment. The foundation for our design environment is the Sandia Analysis Workbench (SAW)--an integrated analysis workflow tool built on the Eclipse framework. SAW contains the key technologies needed for a design environment based on finite element analysis. Among other things, SAW provides the powerful geometry and meshing capabilities from the Cubit product, intuitive analysis input deck creation and editing capabilities, easy to use analysis job submission capabilities tuned for HPC platforms, analysis job progress monitoring and management, and simulation data sharing and management--all wrapped in a professional graphical user interface. Our design environment leverages these capabilities and includes capabilities developed specifically for designing with topology optimization. For example, resulting design surfaces from the topology optimization are extracted in parallel on the HPC platform and returned to the SAW environment for visualization. This parallel extraction on the HPC platform opens the door for “real-time” monitoring of the evolving design surface at regular intervals. Ultimately, the designer will be able to feed the optimization process new constraints and parameters while the optimization is running based on what he sees while monitoring the evolving results. In a real way the user will be in the loop “guiding” the design optimization process to a practical solution. We are confident that this type of user-guided optimization will be critical for successfully providing a powerful and productive design tool based on topology optimization

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Title: Nitsche-Based Cut Finite Element Methods for Multi-Physics Problems

Author(s): Erik Burman, Susanne Claus, Thomas Boiveau, Luke Swift, *U. College London*; Andre Massing, *Umea U.*.

In this presentation, we will discuss our recent advances in stabilised cut finite element methods for multi-physics problems. In the cut finite element method, the interface between two physical domains is allowed to intersect a fixed background mesh arbitrarily. Classically, this type of method suffers from ill-conditioning, when the interface intersects an element close to an element edge or node. The major novelty in our schemes is that we alleviate this major drawback by combining Nitsche's method with so-called ghost penalty terms in the interface region [1]. We demonstrate that the resulting schemes are stable independent of the interface location and that they are consistent and converge with optimal order. In this talk, we will first give a brief review on the basic concepts of Nitsche's method for unfitted or fictitious domain methods [2] and their stabilisation [1]. Then, we will introduce our novel stabilised schemes for a variety of multi-physics problems. In particular, we will present a multi-phase three-field stokes scheme [3], a fluid-structure interaction scheme using a non-symmetric version of Nitsche's method, without penalty term, and a fictitious domain scheme for the Helmholtz problem. [1] E. Burman, S. Claus, P. Hansbo, M. Larson, A. Massing. CutFEM: discretizing geometry and partial differential equations. Int. J. Numer. Meth. Engng, doi: 10.1002/nme.4823, 2014. [2] E. Burman and P. Hansbo. Fictitious domain finite element methods using cut elements: II. Applied Numerical Mathematics 62.4 (2012): 328-341. [3] E. Burman, S. Claus, A. Massing. A Stabilized Cut Finite Element Method for the Three Field Stokes Problem, SIAM J. Sci. Comput., to appear, 2015.

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Title: Using a Sliding Mesh Scheme with Arbitrary Mesh Motion to Simulate the Motion of a Liquid Within a Piston Assembly Subjected to Vibrational Acceleration

Author(s): Jonathan Clausen, John Torczynski, Louis Romero, Timothy O'Hern, *Sandia Nat'l. Lab.*.

We investigate the behavior of a liquid-filled piston assembly that is subjected to vibrational loading. The assembly contains bellows to simulate the presence of air bubbles, and the piston gap contains protrusions such that the geometry of the gap varies due to the piston's motion. Under certain conditions, nonlinearities in the system can produce a large rectified (net) force on the piston. This behavior is investigated using finite element simulations that couple the behavior of the Newtonian liquid to the rigid-body motion of a piston. The bellows are modeled as springs at the domain boundary. The motion of the solid bodies is accommodated using an arbitrary Lagrangian–Eulerian (ALE) approach; however, due to the large piston displacements that occur near the resonance frequency and to the complex geometry, standard ALE techniques break down. Consequently, we combine the ALE technique with a sliding mesh scheme to allow for large displacements of the piston while limiting mesh distortion that occurs with ALE methods. We discuss the numerical formulation of the ALE method and the sliding mesh scheme, and we show simulation results of the piston motion. Also, simulation results are compared with theoretical predictions from a simplified model that was previously developed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Finite Element Approximation of the Two-Phase Viscous-Viscoelastic Flow Problem

Author(s): Ramon Codina, Ernesto Castillo, Joan Baiges, *U. Politècnica de Catalunya*.

In this work we present a finite element model to approximate the equations governing the flow of a viscoelastic fluid moving inside a viscous fluid. It is therefore a two-phase flow of fluids with different rheological behaviour. The complete numerical model consists of several ingredients. The first is a stabilized finite element model for the flow equations. In the case of viscoelastic flows, residual-based stabilization shows a numerical misbehaviour in the presence of singularities. We use instead a term-by-term stabilization based on controlling the projection orthogonal to the finite element space of different terms. This has to be combined with a discontinuity capturing technique, which in our case consists in introducing nonlinear diffusion proportional to the component of the velocity gradient orthogonal to the finite element space [1]. The interphase between the viscous and the viscoelastic components is tracked using a level set method. A classical transport equation is solved for the level set function, which is approximated using a stabilized finite element method and finite difference integration in time. This function is re-initialized get it gets excessively distorted. In order to deal with problems dominated by gravity effects, i.e. low-Froude number problems, we show the importance of enriching the pressure interpolation in the elements cut by the interphase. This enrichment can also be done for the other flow variables, namely, velocity and elastic stress. It consists of a component that is discontinuous between elements and is linear on each side of the interface, so that the gradient is discontinuous. The new degrees of freedom associated to this enrichment can be condensed at the element level, thus maintaining the total number of unknowns of the problem [2]. References: [1] E. Castillo and R. Codina, “Variational multi-scale stabilized formulations for the stationary three-field incompressible viscoelastic flow problem”, Computer Methods in Applied Mechanics and Engineering, Vol. 279 (2014), 579-605 [2] H. Coppola-Owen and R. Codina, “Improving Eulerian two-phase flow finite element approximation with discontinuous gradient pressure shape functions”, International Journal for Numerical Methods in Fluids, Vol. 49 (2005), 1287-1304

13th U.S. National Congress on Computational Mechanics
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Title: Characterizing Damage Using Peridynamics and Digital Image Correlation

Author(s): Johannes Conradie, Thorsten Becker, *U. Stellenbosch*; Daniel Turner, *Sandia Nat'l. Lab.*.

Fracture of structural materials is currently a challenging phenomenon to numerically model as well as experimentally characterize. The peridynamic theory, which is a reformulation of continuum mechanics and bears similarities to molecular dynamics, allows the direct application to cracks. The theory lacks experimental context, where the failure criteria is based on the critical stretch, which is often arbitrarily chosen. Providentially, it can be related to the non-linear critical energy release rate, known as the J-integral from fracture mechanics, however it has rarely been implemented [1]. In this work a peridynamic-based algorithm [2] was implemented using digital image correlation (DIC) full-field displacement measurements combined with the critical energy release rate of a particular material to characterize damage. DIC is a popular optical technique that measures full-field surface displacements of a loaded material and is gaining traction for problems concerned with cracks [3]. In addition, this work aimed to validate the J-integral based failure criterion through the implementation of DIC data. The materials investigated include Polymethyl methacrylate (PMMA), for brittle linear elastic cracking, and both stainless steel 304L and aluminum 1200H4, for elastic plastic deformation. The critical energy release rates and resistance curves of the materials were experimentally obtained through standard ASTM tests on compact tension specimens. The displacement fields and corresponding energy release rates were subsequently implemented into the algorithm. The damage results from the PMMA were accurately revealed near the crack path as compared to the test. Also, the algorithm was able to detect damage caused by plastic deformation of the ductile materials through utilizing the resistance curves. The combination of peridynamics and DIC full-field displacements showed great potential for determining brittle crack damage as well as plastic deformation. This approach can greatly benefit the characterization and detection of structural and component failure due to the initiation of cracks. References 1. Foster, J. T., Silling, S. A. and Chen, W. (2011), ‘An energy based failure criterion for use with peridynamic states’, Journal for Multiscale Computational Engineering 9(6), 675–687. 2. Conradie, J. H., Turner, D. Z. and Becker, T. H. (2014), Characterising damage in structural materials using digital image correlation and peridynamics, in ‘South African Conference on Computational and Applied Mechanics’, Vol. 9, Somerset West, South Africa. 3. Becker, T. H., Mostafavi, M., Tait, R. B. and Marrow, T. J. (2012), ‘An approach to calculate the J-integral by digital image correlation displacement field measurement’, Fatigue and Fracture Engineering Materials and Structures 35(971-984).

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Title: Discontinuous Galerkin (DG) Modified Basis Methods for Baroclinic Flows

Author(s): Colton Conroy, Ethan Kubatko, *Ohio State U.*.

In this talk, we present novel discontinuous Galerkin (DG) modified basis methods for modeling baroclinic flows in the vertical extent of the water column in coastal settings. Specifically, we examine the mean circulation associated with a shallow stratified sea, whose density front is maintained by tidal, wind, or other high frequency mixing. In particular, we develop a novel steady state solution method that utilizes DG spatial discretizations coupled with modified basis methods to solve the problem of interest. All the primary variables, including the free surface elevation, are discretized using discontinuous polynomial spaces of arbitrary order. The difficulty of mismatched lateral boundaries that accompanies the use of a discontinuous free surface is overcome through the use of a so-called sigma coordinate system in the vertical, which transforms the bottom boundary and free surface into coordinate surfaces. The pressure flux that arises from the density variations in the shallow stratified sea is discretized via the DG spatial operator, which serves as a source term for the second-order terms of the boundary value problem. These second-order terms are then discretized with the use of a so-called modified basis method — a method that utilizes a mixed form of the problem along with specific properties of the Legendre polynomials to integrate the discrete source term exactly. The end result is a conservative steady state solution method with preliminary numerical results displaying k + 1 convergence for Pk polynomials up to k = 4.

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Title: Active Subspaces for Dimension Reduction

Author(s): Paul Constantine, *Colorado School of Mines*.

Parameter studies are everywhere in computational science. Complex engineering simulations must run several times with different inputs to effectively study the relationships between inputs and outputs. Studies like optimization, uncertainty quantification, and sensitivity analysis produce sophisticated characterizations of the input/output map. But thorough parameter studies are more difficult when each simulation is expensive and the number of parameters is large. In practice, the engineer may try to limit a study to the most important parameters, which effectively reduces the dimension of the parameter study. Active subspaces offer a more general approach to reduce the study's dimension. They identify a set of important directions in the input space. If the engineer discovers a model's low-dimensional active subspace, she can exploit the reduced dimension to enable other- wise infeasible parameter studies for expensive simulations with many input parameters.

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Title: Carotid Artery Stenting Haemodynamics: A Patient-Specific CFD Analysis

Author(s): Michele Conti, Alessandro Reali, Ferdinando Auricchio, *Pavia U.*; Christopher Long, *Los Alamos Nat'l. Lab.*; Yuri Bazilevs, *UC San Diego*.

The study proposes the analysis of carotid artery haemodynamics before and after stenting using computational fluid dynamics. The study addresses a real clinical case; pre- and post-operative computed tomography images are elaborated to create patient-specific model of the carotid bifurcation. The analysis accounts for an accurate modelling of the endovascular device and of its impact on the local haemodynamics along the arterial bifurcation.

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Title: Stabilization of Nitsche's Method for EFG Analysis of Shear Defformable Shells

Author(s): Jorge Costa, Paulo Pimenta, *U. São Paulo*; Peter Wriggers, *Leibniz U. Hannover*.

Meshless methods such as the Element Free Galerking (EFG) use smooth base functions to approximate field quantities in computational mechanics. This smooth characteristic is especially welcome in shell analysis, where the approximation of displacement and rotations with Moving Least Squares (MLS) provide a smooth initial geometry, primal fields and consequently stress fields. Nevertheless, the lack of a Kronecker delta property in MLS makes the imposition of essential boundary conditions not straightforward. In addition, the resort to a mapped initial configuration turns the solution of kinked shells into a multi-domain problem, where continuity between domains turns into Dirichlet-like conditions. This problem resembles those arising not only from non interpolatory approximations but also from nonconforming meshes, fictitious domain problems and embedded interfaces, using from eXtended Finite Elements to Meshless or Isogeometric approximations. Classically, these impositions (essential boundary condition and interfaces) are enforced through modifications in the weak form, especially using Lagrange Multipliers or Penalty Methods. Recently, the use of the Interior Penalty Method attributed to Nitsche has gained force as a way to avoid new degrees of freedom and a less restricted choice of approximation spaces. Although Nitsche’s method precludes the choice of a new approximation field for the boundary fields, the analysis still includes a penalty-like stabilization parameter, along with a penalty-like term. In this work, we demonstrate that the performance of the method for the analysis of shear deformable shells with EFG is kept for a large range of stabilization constants. We provide separate impositions for displacements and rotations as their different magnitudes may compromise the performance for thin shells. And more importantly, we specify an approach to estimate these parameters for EFG analysis of shells. The formulation is accompanied by several numerical examples where it is demonstrated that the stabilization parameters obtained correspond to the end of the unstable range of stabilization parameters.

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Title: Non-Linear Mechanical Metamaterials

Author(s): Corentin Coulais, *Leiden U.*.

I introduce a novel class of soft porous structures that exhibit elastic instabilities. I use them as a building block to create flexible mechanical metamaterials with highly nonlinear and novel properties, such as negative stiffness, elastic memory and programmability. Combining fabrication via 3D printing, experiments, numerical simulations and theory, I fabricate and investigate the physics of 1D (beams), 2D (holey sheets) and 3D (cubes) systems. On these examples, I will show that elastic nonlinearity is the main ingredient to understand and design these exotic mechanical responses.

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Title: The Inverse Fast Multipole Method as an Efficient Preconditioner for Dense Linear Systems

Author(s): Pieter Coulier, *KU Leuven & Stanford U.*; Hadi Pouransari, Eric Darve, *Stanford U.*.

Linear systems of equations involving dense matrices arise in a variety of applications in science and engineering (e.g., in boundary element methods). Many of these dense matrices can be represented in a hierarchical format, where matrix blocks corresponding to well-separated interactions are replaced by low-rank approximations. Such hierarchical representations facilitate matrix-vector multiplications, hence enabling the use of iterative solvers. The precarious convergence behavior (and thus the number of iterations) is a major disadvantage of this type of solvers, however, depending on the spectral properties of the matrix. This necessitates the incorporation of a preconditioning strategy to improve the latter, which is often a difficult and case-dependent problem. In this talk, the inverse fast multipole method (IFMM) is presented as a robust and efficient preconditioner for iterative schemes involving dense matrices. The preconditioner is essentially a fast direct solver with low accuracy, where "direct" refers to the use of an approximate LU factorization. The solver is inexact, although the error can be controlled and made as small as needed (with an increase in computational cost). The IFMM was originally discussed in [1] and relies on two key ideas. First, the dense hierarchical matrix is converted into an extended sparse matrix, introducing additional unknowns (which can be interpreted as local and multipole coefficients at different levels in the framework of the fast multipole method). Second, fill-ins arising during the elimination of the extended sparse matrix are compressed as low rank matrices if they correspond to well-separated interactions. As a result, the sparsity pattern of the extended sparse matrix is maintained throughout the elimination, resulting in a very efficient algorithm with nearly linear complexity (strictly linear if the rank is bounded independent of the matrix size). The proposed preconditioning strategy shows similarities to multigrid methods [2] (as it uses a hierarchical decomposition of the domain), as well as to the incomplete LU factorization and its variants [3] (as the sparsity pattern is preserved). The IFMM can also be used as an accurate direct solver, although a much higher accuracy for approximating the well-separated interactions is required in that case. References [1] The inverse fast multipole method, S. Ambikasaran and E. Darve, arXiv:1407.1572, 2014. [2] Multi-grid methods and applications. W. Hackbusch, Springer, 1995. [3] Iterative methods for sparse linear systems, Y. Saad, PWS Publishing, Boston, 1996.

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Title: Moving Interfaces in Finite Element Methods: A Fictitious Domain Approach

Author(s): Sebastien Court, *U. Blaise Pascal*.

Addressing PDE problems that involve moving boundaries is a delicate issue since the geometry of the domain can make part of the unknowns and can generate strong nonlinearities. Simulating this kind of situations could lead to consider moving computational domains; Instead of that, we use finite element formulations with a fictitious domain approach for which the boundary does not fit the mesh: The goal is to change the less things we need when the boundary moves through the time. The method we present here has been first introduced in [1] for the Poisson problem and then adapted in [2] for the Stokes problem, and then for Navier-Stokes problem. A first illustration is the unsteady displacement of a solid immersed in a viscous incompressible fluid. An other illustration of this class of methods lies in an algorithmic framework. For instance, for solving numerically an inverse problem, the iterative update of an interface does not necessitate to remesh the whole domain (see [3]). It leads to a gain of time computation and resources. We will take a look at an inverse problem consisting in recovering information (position, shape) on a crack responsible for displacement discontinuities inside a volcano. The data we have are measurements on the surface of the volcano. A gradient algorithm will be presented, dealing with solving direct adjoint problems, and thus underlying the interest of our fictitious domain approach. http://sebastien.court.math.free.fr/ References [1] J. Haslinger and Y. Renard, A new fictitious domain approach inspired by the extended finite element method, SIAM J. Numer. Anal., 47 (2009), no. 2, pp. 1474-1499. [2] S. Court, M. Fournié and A. Lozinski, A fictitious domain approach for the Stokes problem based on the extended finite element method, Int. J. Numer. Meth. Fluids., 74 (2014), pp. 73–99. [3] S. Court, O. Bodart, V. Cayol and J. Koko, XFEM based fictitious domain method for linear elasticity model with crack, in preparation.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: High-Performance Computing for RTM Uncertainty Quantification

Author(s): Danilo Costa, *High Performance Computing Center*; Alvaro Coutinho, .

Characterizations of uncertainties typically require many runs from the seismic computer model where each run is a variation of an incompletely characterized model input. However, RTM can be remarkably computationally expensive, often requiring extensive time on massive supercomputers. The processing cost makes it difficult to study the effects of the parameters on model outputs; thorough sensitivity analysis, uncertainty quantification, and design optimization studies are often infeasible. In that sense, this work assess the computational power needed for uncertainty quantification (UQ) into seismic Reverse Time Migration (RTM), aiming to gain insights about the enabling technology to large-scale analysis. The computational framework presented here regards to a realistic three-dimensional (3D) RTM problem, whose the computational requirements are assessed for both wave equation formulations the acoustic isotropic (ISO) and the Transverse Tilted Isotropy (TTI). Taking into account all calculations performed in a RTM solver, the vast majority of the runtime is spent on computing solutions of the wave equation kernels. Typically, these memory-bound kernels are known to achieve only a low fraction of a processor peak performance, even though significant computational optimizations have been made. Thus, the solver could only explore roughly eight out of thirty-four petaflops per second from the current most powerful supercomputer in the TOP500 list. Given a dataset from a realistic 3D seismic domain with thousands of shot points and given the RTM arithmetic intensity, it is feasible to evaluate the computational cost to process the whole dataset. The results show that dozens of exaflops must to be computed in the case of an isotropic RTM processing, spending near to half an hour running in the TOP500 first machine. For the TTI formulation the runtime achieves tens of hours. Indeed, running the RTM uncertainty quantification in a supercomputer with one petaflop/s, the computational cost could become prohibitive. Intensive performance improvements must be developed in the UQ realm in order to allow a robust RTM analysis. Is expected to take seismic UQ analysis to a new level using Exascale computing resources that will likely come from accelerator-based, many-core architectures.

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Title: Towards Extreme Computing for Uncertainty Quantification in Seismic Imaging

Author(s): Leonardo Borges, *Intel*; Danilo Costa, Thibaut Lavril, Luciano Leite, Thomas Miras, Marta Mattoso, Fernando Rochinha, Vitor Souza, *Federal U. Rio de Janeiro*; Alvaro Coutinho, *Federal U. of Rio de Janeiro*; Josias Silva, *PETREC*.

This paper presents a progress report on our project within Intel® Parallel Computing Centers (Intel® PCC) program, focused on improving seismic imaging for oil and gas exploration. Seismic imaging can be viewed as an application area where extreme scale computing always has been of fundamental importance. This is on the forefront of HPC and Parallel Computing, exhausting available resources on large clusters, usually equipped with coprocessors, such as Intel® Xeon Phi™ Coprocessor. Seismic simulations require fine-tuned codes and extensive optimization, given the enormous amount of required processing time and data generated in marine seismic surveys. Recently another complexity layer has been added, the uncertain character of the underlying mathematical models. This has the potential to increase manifold not only the computational effort to generate the uncertainties in the images, but also the data, since several runs will be necessary to sample with a proper method the stochastic space. Key to the success of this new strategy is highly optimized codes, making use of the utmost techniques in code optimization and tuning, parallel I/O and related enabling technologies on managing the execution of hundreds of jobs on large clusters. The paper will start discussing a possible uncertainty quantification (UQ) scenario for Reverse Time Migration - an imaging algorithm widely used in the oil industry. In the sequel we will show improvements in stencil computations for Intel® Xeon Phi™ Coprocessor, that will affect overall computational performance. The UQ scenario will be modeled as a scientific workflow. We will then explore Chiron, an algebraic parallel scientific workflow engine, to monitor and steer such UQ computations. Issues such as the importance of runtime provenance support, fault tolerance, file systems, parallel databases arise naturally in this context. Proof-of-concept computations at Intel's clusters will be shown to support our claims, pointing on how to best explore these technologies on extreme computing environments.

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Title: Fluid-Structure Interaction Using Immersed Boundaries and Geometrically-Exact Beam Theory with Contact

Author(s): Paulo M. Pimenta, Henrique C. Gomes, Luiz Couto, Alfredo Gay Neto, *U. São Paulo*.

This work deals with a class of fluid-structure interaction problems in which the structure can move with large displacements including contact interaction with other bodies or itself. The structure is modeled using geometrically-exact rods, including the possibility of contact interaction with rigid walls representing the boundary of the desired physical domain. Furthermore, self-contact searching is also addressed for particular situations when the structure tries to touch itself. Both contact with the walls and self-contact consider large displacements possibility, including normal and friction effects using a penalty approach. The interaction between fluid and structure domains is solved by an immersed boundary approach that uses discontinuous Lagrange multipliers to enforce kinematic and force equilibrium along the interface between the non-matching overlapping meshes, in an alternative to usual Arbitrary Lagrangian Eulerian (ALE) approaches. The engineering applicability of the proposed work is of great interest to deep water offshore oil exploitation. Risers structures usually are subjected to sea current effects and many important phenomena such as vortex induced vibration (VIV) is a result of fluid-structure interaction. The proposed technique uses few elements to solve the structural problem, once structural rod elements are considered. Bi-dimensional unsteady flow of an incompressible viscous fluid is adopted, and the interaction with the structural model is enforced by a separate solution of structure and fluid problems, connected by loading and displacements updating during simulation, step by step, along a dynamic transient time evolution.

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Title: The Flux Reconstruction Method for Solving Unsteady Incompressible Navier-Stokes Equations with Implicit Time Stepping on Unstructured Grids

Author(s): Christopher Cox, Chunlei Liang, Michael Plesniak, *George Washington U.*.

We report the development of an efficient high-order flux reconstruction method for solving the unsteady incompressible Navier-Stokes equations on unstructured grids. With the development of high-order unstructured methods comes the need to achieve faster convergence, especially for solving large-scale problems. This demand motivates the development of time stepping techniques for which the CFL condition is less restrictive, which is hardly the case when explicit schemes are combined with high-order methods. We choose to employ Chorin's classical artificial compressibility treatment of the governing equations for unsteady flow, where dual time stepping is required. With the introduction of artificial compressibility the pressure and velocity are coupled and the Navier-Stokes equations take on a mixed hyperbolic/parabolic mathematical nature. This permits the adoption of advanced time stepping techniques used for solving compressible flow problems. Therefore, a lower-upper symmetric Gauss-Seidel (LU-SGS) scheme with backward Euler discretization is used to efficiently march the solution in pseudo time, while a second order backward Euler discretization is used to march in physical time. As computers become equipped with larger RAM, implicit time stepping schemes are seen as effective drivers to overcome stiffness associated with the artificial compressibility approach, especially for flows that require high aspect ratio elements near solid walls. With these implicit schemes much larger time steps can be taken when compared to explicit schemes, delivering the potential to improve the rate of convergence significantly. In recent years, the LU-SGS scheme has been utilized within the high-order CFD community for solving compressible flow problems on unstructured grids. However, when solving incompressible flows, the LU-SGS scheme is more economical because we require the solution of only three equations (in 2D) as opposed to four equations for compressible flow. We demonstrate order of accuracy with steady Taylor-Couette flow. We further validate the solver with steady flow past a NACA-0012 airfoil at zero angle of attack and unsteady flow past a circle. The implicit time stepping scheme is proven efficient and effective for driving the pseudo time derivative term toward zero in the classical artificial compressibility formulation. As a result, this scheme is capable of quickly establishing the divergence-free velocity condition of the continuity equation when compared to an explicit third order three-stage Runge-Kutta scheme.

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Title: Identification of a Cohesive Law Under Mode-III Conditions

Author(s): Gabriele Cricrì, Michele Perrella, *U. Salerno*; Salvatore Sessa, *U. Napoli Federico II*; Nunziante Valoroso, *U. Napoli Parthenope*.

A method is presented for studying bonded assemblies under pure mode III loading. It is based upon a novel fixture that can be mounted on a common universal testing machine and is able of realizing pure anti-plane shear conditions. Twisting of the bonded assembly generates a smoothly propagating circular crack front that allows for accurate measurements during the test. Data reduction is carried out based on the global load-displacement response and material properties are identified. Results are presented that demonstrate the capabilities of the proposed approach to provide the mode III fracture parameters and the relevant cohesive relationship for adhesively bonded assemblies. REFERENCES [1] G. Cricrì, M. Perrella, S. Sessa, N. Valoroso, 2015, A novel fixture for measuring mode-III toughness of bonded assemblies, in press.

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Title: Dislocation Dynamics Simulations of Void Strengthening Mechanisms

Author(s): Joshua Crone, Lynn Munday, Jaroslaw Knapp, *US Army Rsch. Lab.*.

Material defects alter the evolution of dislocations by directly impeding motion and perturbing the homogenous elastic fields of the bulk crystal. The small scale plasticity occurring in the vicinity of crystal defects is dependent on the motion of individual dislocations and is therefore well suited for discrete dislocation dynamics (DDD) methods where plasticity is explicitly captured by the motion of dislocations. In the last two decades, multiple analytical and numerical methods have been developed in attempt to incorporate the complex stress fields due to microstructure and free surface effects. However, modeling realistic length scales, time scales, and microstructure has shown to be intractable with current DDD algorithms. In this work, we develop a scalable algorithm for modeling DDD with microstructural effects. The method involves coupling a highly parallel DDD simulator for bulk materials (ParaDiS) with a highly parallel finite element method (FEM) solver to capture microstructual effects. Using a scalable data transfer algorithm, we are able to independently control the domain decomposition and computational resource allocation of each application to enable orders of magnitude increases in tractable system sizes. In the present work we use the DDD-FEM code to simulate dislocations interacting with voids. Irradiation-induced and processing-induced voids have been shown to increase the yield and flow stress of materials by restricting dislocation glide. However, current void strength models have been unable to accurately account for the image forces acting on the dislocation due to the void's free surface. We show that image forces significantly reduce the critical strength for a dislocation to bypass an array of voids and present a new model relating critical stress to void size and spacing. We also perform large scale simulations with random distributions of voids and dislocations to determine the effect of porosity on yield and flow stress.

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Title: A 3D Meso-Scale Model to Describe the Mechanical Effects of the Alkali-Silica Reaction in Concrete

Author(s): Aurelia Cuba Ramos, Cyrille Dunant, Jean-François Molinari, *EPFL*.

The alkali-silica reaction (ASR) is one of the most common causes of internal degradation in massive concrete structures like dams. During the reaction, amorphous silica, contained in the aggregates, transforms into an expansive silica-gel. The gel starts swelling by adsorbing water and therefore induces internal stresses in the concrete which then lead to micro-cracking. Macroscopic effects of ASR include an expansion of the structure, cracking, and sometimes spalling. Mechanically, this can be quantified by a loss of strength and elastic modulus. The reaction thus impacts the serviceability and safety of the structure, especially at later stages. Reliable numerical models are required to accurately predict the long-term evolution of ASR. Such models can then be used to design possible rehabilitation measures. The chemical reaction, i.e. the gel formation, is complex and depends on various parameters, such as the environmental conditions. However, it has been shown in previous studies that the mechanical consequences of ASR can be separated from the chemical process [1,2]. For the mechanical response it only matters how much gel is present at each step of the analysis, if creep is neglected. In this work we present a 3D meso-scale model based on this assumption. The cement matrix, the aggregates, and the expansive gel are modeled as separate phases and a continuum damage approach is used to model the complex crack networks. The results obtained show how cracks initiate around the gel sites, propagate through the aggregates and spread into the paste. Furthermore, the model allows to study the influence of different loading conditions. This is of particular importance because real concrete structures are always exposed to external loads. The results suggest that the expansion is not redistributed but that the crack orientations change with the direction of the external loads as previously observed in [3]. Finally, we provide an outlook on how this model can be upscaled to perform macroscopic simulations of ASR affected structures. [1] M. Ben Haha, E. Gallucci, A. Guidoum, K. Scrivener. Relation of expansion due to alkali-silica reaction to the degree of reaction measured by sem image analysis. Cem. Conr. Res. 37(8) (2007). [2] C. Dunant. Experimental and modelling study of the alkali-silica reaction in concrete. PhD thesis, Ecole polytechnique fédérale de Lausanne (2009). [3] C. Dunant, K. Scrivener. Effects of uniaxial stress on alkali-silica reaction induced expansion of concrete. Cem. Conr. Res. 42(3) (2012).

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Title: Solution of a Robust Optimization Problem to Maximize the Rate of Penetration of Horizontal Drillstrings Using a Non-Linear Stochastic Dynamic Model

Author(s): Americo Cunha Jr, *U. Estado do Rio de Janeiro*; Christian Soize, *U. Paris-Est*; Rubens Sampaio, *PUC-Rio*.

A drillstring is a long column under rotation, composed by a sequence of connected drill-pipes and auxiliary equipment, which is used to drill the soil in oil prospecting. During its operation, this column presents a three-dimensional dynamics, subjected to longitudinal, lateral, and torsional vibrations, besides the effects of friction, shock, and bit-rock interaction. Due to the relevance of this equipment in some engineering applications, this work aims to analyze the nonlinear dynamics of drillstrings in horizontal configuration. A computational model, which uses a nonlinear beam theory of Timoshenko type that takes into account the coupling between longitudinal, transverse, and torsional vibrations, is considered. This model also takes into account the effects of friction and shock, induced by the lateral impacts between the drillstring and borehole wall, as well as bit-rock interaction effects. The uncertainties of the bit-rock interaction model are taken into account using a parametric probabilistic approach. Numerical simulations have shown that the mechanical system of interest has a very rich dynamics, which reproduces phenomena such as bit-bounce, stick-slip, and transverse impacts. Two optimizations problems (one deterministic and one robust), where the objective is to maximize the drillstring rate of penetration (ROP) into the soil, respecting its structural limits, are formulated and solved. In order to optimize the ROP, it is possible to vary the drillstring velocities of translation and rotation. The solutions of these optimization problems provided two different strategies to maximize the ROP.

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Title: Concurrent Multi-Scale Modeling: From Quantum to Continuum

Author(s): W. A. Curtin, *EPFL*.

Concurrent multiscale modeling can be essential for the accurate study of some problems where either (i) the fields are long-range (e.g. cracks or dislocations) or (ii) important coupled phenomena are occurring at several scales simultaneously (e.g. plasticity or diffusion). Here, we present three recent developments addressing the bridging of length and time scales, and focus on key elements of the coupling method/algorithm rather than on applications. First, we briefly discuss a new Quantum/Atomistic coupling method for accurately embedding a fully Kohn-Sham density functional theory (DFT) domain within a surrounding atomistic domain [1]. The key new concept is that of “constrained DFT” wherein constraints on the electron density on the outer boundary of the DFT cell are imposed to match the bulk electron density. Second, we present recent progress in the formulation of fully-dynamic atomistic/continuum coupling at finite temperatures using force coupling [2]. A new finding is that force coupling is dynamically unstable due to any mismatch in the non-linear description of the material across the atom/continuum interface. However, strategies to mitigate this problem are identified and demonstrated. Third, we present a new multi-time scale approach in which a large scale diffusion problem is coupled to an explicit fully-atomistic region to model the evolution of crystal defects due to absorption of point defects via diffusion [3]. The atomistic dynamics is handled by accurate accelerated molecular dynamics methods, with far-field diffusion evolving as the defect itself evolves in structure. Finally, we provide a brief update of progress in the “Coupled Atomistic/Discrete-Dislocation” method in both 2d (plane strain) [4], 3d, and an implementation of the coupling method within LAMMPS (presented fully in another presentation) [5]. 1. X. Zhang, G. Lu, and W. A. Curtin, Phys. Rev. B 87, art. #054113 (2013). 2. T. Junge, G. Anciaux, J. F. Molinari, submitted (2014). 3. K. L. Baker and W. A. Curtin, submitted to MSMSE (2015). 4. S. Chakravarty, B. Szajewski, and W. A. Curtin, in preparation. 5. F. Pavia and W. A. Curtin, submitted to MSMSE (2014).

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Title: Proper Orthogonal Decomposition Model Reduction for the Explicit Solution of Large Discrete Systems

Author(s): C. Ceccato, *U. Padua*; X. Zhou, D. Pelessone, G. Cusatis, *Northwestern U.*.

The use of explicit dynamic algorithms for computing the quasi-static response of large highly nonlinear discrete systems, although extremely beneficial as far as convergence issues are concerned, may become impractical in terms of computational time due to time step stability requirements. Various solutions have been investigated in literature to overcome this problem and an interesting approach can be found in the Proper Orthogonal Decomposition (POD) as a model reduction technique. In this study, the computational framework for the explicit integration of the dynamics equations of motion through POD is proposed with particular reference to large discrete systems and a low dimensional approximation of the complete system response is generated by the so-called Proper Orthogonal Modes, computed with snapshots from the complete simulation. Aiming to the formulation of an adaptive framework, the Proper Orthogonal Modes are calculated in itinere, during the analysis itself, alternating the integration in the complete system, for the snapshots collection, with the integration in the reduced system, until the modes previously collected provide a good representation of the response. Numerical details relevant to the transition between the complete and the reduced system (and vice versa) as well as issues with imposing essential and natural boundary conditions are discussed. The performed numerical simulations show that for both linear and nonlinear behavior, just few modes are capable of excellent approximation of the complete solution, allowing to conveniently (a) reduce the size of the problem in terms of degrees of freedom and (b) increase the critical time step of the simulation without significant loss in accuracy.

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Title: IMEX Lagrangian and ALE Methods for Multiphysics Systems

Author(s): Eric C. Cyr, *Sandia Nat'l. Lab.*.

An appealing methodology for simulating multiphysics shock-hydro systems is the Arbitrary Lagrangian Eulerian (ALE) method. One approach is to implement this using an operator splitting type-procedure: (1) take Lagrangian step following the advected/pressure wave time-scale, (2) remesh and remap physical quantities, and (3) solve for the remaining physics on the remapped mesh. This approach has been successful in many practical applications of interest. However, for multiphysics regimes characterized by multiple interacting time and spatial-scales this splitting may have stability limitations that force the time step to be too small to efficiently follow the time scales of interest. An alternative formulation to ALE is to solve the system monolithically. For explicit time stepping this approach may have similar challenges with disparate and overlapping time-scales. Additionally fully implicit solution methods may ultimately be deemed too costly because of the expense and challenge of solving large-scale multiphysics systems. An appealing approach to resolve these issues is to develop an Implicit-Explicit (IMEX) time stepping formulation of the monolithic ALE equations. IMEX schemes are mathematically well-structured approaches that permit the separation of timescales within a fully coupled residual formulation. These methods support the development of high-order in time integration methods and adjoint methods for sensitivity analysis, both of which can be challenging in the operator-split regime. This talk will review the structure of IMEX Runge-Kutta schemes. These time integrators will be applied to a VMS stabilized Lagrangian formulation of the Euler equations. We will also present results demonstrating the feasibility of a monolithic multiphysics ALE scheme using IMEX time integrators.

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Title: Modeling and Simulations of Liquid-Liquid Immiscible Flow Through Heated Microchannels

Author(s): Antonio da Cruz, Gabriel Guerra, Fernando Duda, *U. Federal Rio de Janeiro* .

Two-phase flows of immiscible liquids appear in the context of several applications. For instance, flows involving droplets and slugs have the potential of enhancing heat transfer in microfluidic devices. Whereas standard treatments of these flows consider the interfaces between phases as surfaces of discontinuity, phase-field models considers that the different phases are separated by three-dimensional transition zones across which the fields and material properties that characterize the bulk phases vary smoothly. In this work we develop a non-isothermal phase-field model thermodynamically consistent for studying two-phase flows of immiscible fluids. Further, the model is applied to perform numerical simulations of non-isothermal droplet or slugs flows in microchannels. Our goal is to get insight on the dynamics of droplets or slugs moving in microchannels in order to enhance the heat transfer in microfluidic devices. On the side of numerical method, we discretize the non-isothermal two-phase hydrodynamic model using a C0-stabilized finite element formulation, which increases the stability of the pressure variable and avoids some drawbacks of the standard Galerkin approximation. Numerical simulations of two-phase incompressible flows are computed and found to be in good agreement with existing numerical studies in the literature. We examine the influence of the coupling terms in the governing equations and parameters such as flow rate ratio, viscosity ratio, and interfacial tension of drops in immiscible fluids.

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Title: Representing the Earth's Surface with a Spherical Tessellation in Satellite Based Remote Sensing Simulations

Author(s): Keith Dalbey, Daniel Arpin, Matthew Martin, Ronald Shaw, *Sandia Nat'l. Lab.*.

Satellite based remote sensing is useful for measuring how quantities, such as temperature, are distributed over the Earth's surface, particularly when certain regions of the Earth are physically inaccessible. Simulations of existing or proposed satellite constellations are often used to assess or predict aspects of system performance including the degree, accuracy, and reliability of sensor coverage. Global metrics, such as the mean global temperature are also common in contexts such as climate simulations. This talk describes a C++ spherical tessellation class which is being used at Sandia National Laboratories to represent the Earth's surface in a simulator of satellite based remote sensing performance. This tessellator is capable of: measuring the quality of arbitrary sample designs embedded on the surface of a sphere and comparing that to the theoretically optimal value of the quality metric; generating optimal spherical Centroidal Voronoi Tessellation (CVT) designs; spatial integration which for those CVTs is provably optimal for C2 continuous functions; highly accurate integration error estimates for functions that are C2 continuous, piecewise constant, or have intermediate degrees of smoothness; generating "heat maps" in linear time via either piecewise linear or piecewise constant interpolating from values at arbitrary points; and adaptive mesh refinement based on either geometry or the previously mentioned error estimates. Note that although the tessellation is generated using a spherical Earth assumption, the distance between sample points and the center of the Earth can be subsequently adjusted to other Earth approximations, for example WGS84. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Effect of Silicon Morphology on Mechanical Stability of Si-CNT Heterostructure Anode Configuration for Li-Ion Battery

Author(s): Sameer Damle, SIladitya Pal, Rigved Epur, Prashant Kumta, Spandan Maiti, *U. Pittsburgh*.

In order to improve the capacity of Li-ion batteries to fulfill the ever-increasing energy demands of high performance electronic devices, silicon has emerged as the forerunner to replace the traditional graphite anodes (~372 mAh/g) due to their superior specific capacity (~4200 mAh/g). However, the colossal volumetric expansion of Si (~300%) during its electrochemical cycling leads to its mechanical degradation causing loss of electronic conductivity and anode capacity. On the other hand, carbon nanotubes (CNTs) are known to have very good mechanical strength along with excellent electrical and thermal properties. Thus, a heterostructure comprising of CNT core and nanostructured Si shell can combine merits of both these structural elements by capitalizing on physical and electrochemical properties of CNTs and Si to give improved capacity retention. The electrochemical cycling results shown by Epur et al.[1] illustrate that the Si-CNT heterostructure with nano-particulate morphology of Si outperforms the Si thin film morphology. This indicates that the morphological features of Si in the heterostructure can significantly alter the anode performance. However, mechanistic understanding of this observation is required to further improve the Si-CNT heterostructure anode performance. Focus of the current study is to understand the effect of Si morphology in the Si-CNT heterostructures on its mechanical integrity during electrochemical cycling. We utilize a thermodynamically consistent multiphysics modeling framework developed by us[2] that accounts for Li diffusion induced large deformation in the heterostructure anode, elasto-plastic deformation of the lithiated Si, as well as the failure occurring in different Si/CNT heterostructure anodes configurations. This framework is employed in a nonlinear finite element framework to compare different Si-CNT heterostructure morphologies in terms of their mechanical durability during electrochemical cycling to identify the most stable Si/CNT electrode configuration. Fracture at the CNT/Si interface is modeled using a novel cohesive law[3] that accounts for the fracture strength and toughness of the interface. Two-phase lithiation of the amorphous Si is considered. Comparison of simulation and relevant experimental results will be presented and discussed. Results from this study are expected to aid in the fabrication of improved Si/CNT heterostructure anodes. 1. Epur, R., et al., Electrochimica Acta, 2012. 85: p. 680-684. 2. Pal, S., et al., Journal of Power Sources, 2014. 246: p. 149-159. 3. Ortiz, M. and A. Pandolfi, International Journal for Numerical Methods in Engineering, 1999. 44: p. 1267-1282.

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Title: Advances in Second-Order Finite Elements for Explicit Methods in Non-Linear Solid Dynamics

Author(s): Kent Danielson, *U.S. Army Engineer Rsch. & Dev. Center*.

The authors present some recent developments that build on the previous second-order 27-node hexahedral elements developed for explicit methods in nonlinear solid dynamics [1]. These include the development of second-order 15-node tetrahedral [2] and 21-node wedge elements for explicit methods, an alternate simple pressure-projection method for incompressibilities, and strategies for improved critical time increment predictions. The primary motivation for the development of the tetrahedral and wedge elements is to be able to utilize simpler all-Tet or Hex-Dominant meshing software. Several basic explicit dynamic formulations were shown to be viable for general applications, specifically “full” Gauss for compressible materials as well as selectively reduced Gauss integration and a lowered-order pressure-projection method for nearly incompressible materials. Satisfactory performance was found in standard benchmark problems as well as in large practical applications using various hyperelastic and inelastic material models and involving very large strains/deformations, severe distortions, and contact-impact. As found for the 27-node bricks, row summation lumping, Lagrange interpolants, and high-order Gauss quadrature rules were shown to be crucial for reliable explicit analyses. Results of a rigorous examination of the influence of distortion and material properties on individual elemental eigenvalues are used to show their effects on the computation of the critical time increment. In many cases, the reliable formulations were computationally expensive, but they were found to be competitive with other element types, particularly in bending, and without using either hourglass control or incompatible modes. They are still practical for large applications, especially using today’s parallel computers, and especially, are amenable to more automatic and easier to use meshing strategies. References [1] K. T. Danielson and J. L. O’Daniel. Reliable second-order hexahedral elements for explicit methods in nonlinear solid dynamics. Int. J. Numer. Meth. Engng 2011; 85(9):1073–1102. DOI: 10.1002/nme.3003. [2] K. T. Danielson. Fifteen node tetrahedral elements for explicit methods in nonlinear solid dynamics. Comput. Methods Appl. Mech. Eng; 272:160-180. DOI: 10.1016/j.cma.2014.01.012 Acknowledgments: Permission to publish was granted by Director, Geotechnical and Structures Laboratory. The work was supported in part by grants of computer time from the DOD High Performance Computing Modernization Program at the ERDC DoD Supercomputing Resource Center (DSRC).

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Title: Modeling Dynamic Shearing Deformations In Living Human Brain with Relevance to Traumatic Brain Injury

Author(s): Nitin Daphalapurkar, Shailesh Ganpule, *Johns Hopkins U.*.

Diffuse Axonal Injury (DAI), a devastating type of Traumatic Brain Injury (TBI) due to closed-head trauma, is the most common debilitating injury that leads to instantaneous unconsciousness and affects millions of people in the United States every year. DAI is a primary type of injury, meaning the injury to the axons occurs at the time of the accident as opposed to other secondary factors associated with the injury (e.g. swelling), which are delayed in time. A leading mechanism of DAI is an injury-causing deformation of an axon, leading to its dysfunction. The exact degree and extent of microscopic injuries are almost impossible to diagnose in vivo using existing imaging modalities, including magnetic resonance imaging. Material point method (MPM) computational simulations were used to predict dynamic deformations in a person-specific brain subjected to mild rotational accelerations. Data on the anatomy of the human head and fiber substructure in the white matter of the brain was obtained from MRI and DTI techniques, respectively. A simplified form of Holzapfel-Gasser-Ogden model was used as the constitutive model for the brain tissues. The material model for white matter further considered fibrous-substructure and viscoelasticity associated with the white matter tissue. Constitutive model for white matter was calibrated based on literature-reported mechanical responses. Cerebrospinal fluid was modeled as a non-Newtonian fluid. MPM is naturally capable of modeling solid-fluid interactions. The results from computations were validated against deformations from in vivo experiments using tagged MRI. Results suggest the contribution to local shearing strains in the axonal-regions of the brain (white-matter for the most part) might occur when the head is violently accelerated or decelerated. The dynamics associated with the shear wave propagation can further amplify the local shearing strains in the brain tissue. The validated human head model was further used to simulate an injury-causing rotational head acceleration, which demonstrates the ability of the computational head model to predict the likelihood of injury, the locations of injury, and likely cognitive dysfunctions.

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July 27-30, 2015, San Diego, California, USA

Title: Mixed Convolved Action for Computational Dynamic Thermoelasticity

Author(s): Gary Dargush, Bradley Darrall, *SUNY Buffalo*.

Considerable effort has been directed in recent years toward the development of variational methods and computational algorithms for the dynamics of conservative systems. On the other hand, the development of true variational formulations for irreversible processes remains a challenge. In this paper, we consider variational methods for the linear dynamical response of thermoelastic solids, based upon extensions of the recently developed concept of mixed convolved action [1,2]. This new formulation uses mixed impulsive variables, fractional calculus and the convolution of convolutions. Remarkably, the stationarity of the mixed convolved action provide the governing partial differential equations of dynamic thermoelasticity, along with all of the initial and boundary conditions of the problem, as the corresponding Euler-Lagrange equations. For the sake of generality, we formulate the theory for fully coupled thermoelasticty with second sound and then explore time and space finite element methods to solve the associated initial/boundary value problems. For the non-dissipative case, these are symplectic, energy conserving numerical algorithms, while in the non-conservative case these approaches provide variationally consistent solutions. Several computational examples are studied to verify the numerical implementation and to explore interesting aspects of non-classical thermoelasticity. References [1] G.F. Dargush, J. Kim, Mixed convolved action, Physical Review E 85 (2012) 066606. [2] G.F. Dargush, Mixed convolved action for classical and fractional-derivative dissipative dynamical systems, Physical Review E 86 (2012) 066606.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Mixed Finite-Element Method for Size-Dependent Piezoelectric Dielectrics

Author(s): Bradley Darrall, Ali Hadjesfandiari, Gary Dargush, *SUNY Buffalo*.

Classical continuum mechanics does not predict well the behavior of materials at very small length scales. This provides the primary motivation for developing a size-dependent continuum theory, such as the linear, isotropic couple-stress theory we consider here as the basis for studying multi-scale, multi-physics phenomena. In this couple-stress theory, there is a new material property with the dimensions of length. Inclusion of couple-stress effects only becomes critical for characteristic geometry on the order of that length. Recent advances in couple-stress theory have solved many of the problems that previous size-dependent continuum theories have had. Some of the more important discoveries relate to the skew-symmetric nature of the couple-stress tensor and the establishment of mean curvature as the correct measure of deformation, as opposed to the strain-gradient [1]. Based on the recent advances in couple stress theory, here we develop a corresponding mixed finite element formulation. Due to the higher order of the governing equations, it would seem that we need to maintain C1 continuity. However, this continuity requirement is satisfied by developing a mixed formulation in which rotations are considered independent of displacements, and then constrained by the use of Lagrange multipliers. It is shown that this formulation has the distinct advantage that these Lagrange multipliers are actually equal to the skew-symmetric portion of the stress tensor, which makes evaluating the stress field a simple task. In addition, we consider the extension of linear isotropic couple-stress theory to include electro-mechanical coupling between the curvature and electric fields. This is known as flexoelectricity [2] or size-dependent piezoelectricity [3]. From classical piezoelectric theory, we know that isotropic materials cannot exhibit linear electro-mechanical coupling that occurs between strain and electric fields. However, it is interesting that if we consider coupling between the electric and curvature fields, then we find that size-dependent effects can be present, even in isotropic materials. We show that extending the finite element formulation presented here to include these size-dependent piezoelectric effects is quite straightforward. Finally, we apply this new couple-stress finite element formulation to several computational examples to validate the numerical implementation and to explore electromechanical couplings. References [1] A.R. Hadjesfandiari, G.F. Dargush, Couple stress theory for solids, International Journal of Solids and Structures, 48 (2011) 2496-2510. [2] A.K. Tagantsev, Piezoelectricity and flexoelectricity in crystalline dielectrics, Physical Review B, 34 (1986) 5883-5889. [3] A.R. Hadjesfandiari, Size-dependent piezoelectricity, International Journal of Solids and Structures, 50 (2013) 2781-2791.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Random Matrix-Based Stochastic Upscaling for Nonlinear Finite Deformation Behavior

Author(s): Sonjoy Das, Sourish Chakravarty, *U. Buffalo*.

In this work, a physics-based stochastic upscaling scheme is proposed to account for the effects of “mesoscale material uncertainties” in the macroscopic nonlinear constitutive material properties by duly respecting the fundamental physical principles and constraints. The proposed work relies on random matrix theory that has recently been successfully applied to characterize the model-form errors in computational mechanics field. Here, a structural system of interest is conceptually envisaged as characterized by two distinct length scales: a mesoscale regime (0.001 mm to 1 mm) which includes micro-structural features along with micro-anomalies, micro-inclusions, and micro-cracks (~ 0.1 mm or less), and a macroscopic regime (>>1 mm) which alludes to the original structural system that must be modeled in silico by incorporating the effects of micro-structural information. It is envisioned that the link between mesoscale and macroscale are two matrix-valued bounds of the macroscopic constitutive properties that can be determined by applying variational argument on a small mesoscale material volume element that is less than the size of a classical representative volume element. The proposed work is illustrated by determining these matrix-valued bounds (in the positive-definite sense) for nonlinear finite deformation elastic material behavior by considering a certain macroscopic instantaneous tangential constitutive symmetric 9-by-9 matrix that relates the conjugate pair of the nominal stress tensor and the deformation gradient tensor.

13th U.S. National Congress on Computational Mechanics
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Title: Thermal Conductivity of Recycled Asphalt Pavement Particles

Author(s): Eshan Dave, *U. New Hampshire*; Christopher DeDene, *Wisconsin Dept. Transport*.

The bulk thermal conductivity of asphalt mixture and recycled asphalt pavement (RAP), that is, the thermal conductivity of a composite material consisting of asphalt binder, aggregates and air can be readily measured in laboratory. In order to obtain the individual material properties, back calculation with numerical modeling was employed. By modeling the experimental set-up, it was possible to vary the properties of the individual particles to replicate the results of the laboratory testing. Many finite element iterations were run using the data gathered from the experiments to determine extract the particle properties based on the global response of the system. This resulted in known material properties for the individual particles, rather than the bulk properties. Using the thermal conductivities of the individual particles, it was then possible to simulate spherical particles coated in layers of asphalt to obtain the thermal conductivity of the aged asphalt binder contained on the RAP. From this research a few conclusions can be reached. Using a model for the laboratory testing, the bulk thermal conductivities obtained from experimentation were successfully converted into a material property for the three types of specimens tested. Building on the simulated material properties, a method for determining asphalt binder film thickness was developed. This method consisted of simulating one sphere of aggregate coated with asphalt binder, then back calculating the thermal conductivity of the asphalt layer. The back calculated thermal conductivity of the asphalt binder was then used to estimate the asphalt binder thickness. For large particles, the back calculated binder thickness was an acceptable thickness, however as smaller particles were tested, the asphalt binder thickness must increase, as shown by finite-element simulation and with the generalize self consistent scheme model (GSCM). This finding contradicts conventional assumptions of a uniform binder thickness on aggregates.

13th U.S. National Congress on Computational Mechanics
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Title: Finite-Element Simulation of Asphalt Drum Plant

Author(s): Eshan Dave, *U. New Hampshire*; Christopher DeDene, *Wisconsin Dept. Transport.*.

Using ANSYS, a virtual asphalt mixing drum was created. Utilizing thermal symmetry, only a sub section of an entire drum was created. In order to reduce computational time, rather than passing a moving particle through a rotating drum the assumption was made that only the heating due to superheated interstitial would heat the particles inside the drum. With this assumption, it became possible to fix the drum and the particle inside the drum, but allow the inlet temperature of the drum to vary. This would mimic the range of temperatures the particle would experience inside of an actual drum, but save on computational time since mixing would not be simulated. Three different types of analysis were performed, one on pure aggregates, a second on homogeneous reclaimed asphalt pavement (RAP) particles, and the third on aggregates coated in asphalt, which was referred to as a composite. All of the simulations had a linear drum temperature profile, which started at either 500°F for pure aggregates or 400°F for cases with asphalt. The outlet temperature for all simulations was fixed at 300°F. The results of the aggregate heating showed that taconite aggregate possess more desirable thermal properties for asphalt pavement recycling than conventional aggregates. According to the literature, the heat contained in the aggregates contributes to the heating and melting of the asphalt binder contained in RAP. Since the taconite becomes hotter faster, this aggregate would carry more heat to the RAP. A secondary benefit of the higher thermal conductivity of the taconite is that the heat contained in the aggregate will be transferred out of the aggregate faster than with traditional aggregates, which may improve the time needed to heat RAP. Simulations with pure asphalt binder showed that smaller particles were heated faster than larger ones, but in both cases the particles failed to reach the recommended mixing temperature range within 10 seconds of entering the drum. Composite RAP particles with a taconite center were shown to heat faster than particles made of conventional aggregates; however the composite particle failed to heat as fast as a homogenous particle of RAP.

13th U.S. National Congress on Computational Mechanics
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Title: Comparison of Several Staggered Atomistic-to-Continuum Concurrent Coupling Strategies

Author(s): Denis Davydov, Jean-Paul Pelteret, Paul Steinmann, *U. Erlangen*.

The atomistic and continuum descriptions of matter are concurrently coupled in a staggered manner. The continuum-to-atomistic link is implemented using an affine assumption for the outer region of the atomistic description, where the ions are fully enslaved to the continuum solution. The atomistic-to-continuum link is based on fields that are calculated from the atomistic solution [1]. It utilizes the atomistic-to-continuum correspondence, obtained by spatial averaging in the spirit of Irving and Kirkwood, and Noll. In this work, different mechanisms to pass the information from the atomistic domain to continuum are studied [2]. The schemes considered here are decomposed into the surface-type (displacement or traction boundary conditions) and the volume-type. The latter restrict the continuum displacement field (and possibly its gradient) in some sense to the atomistic (discrete) displacements using Lagrange multipliers. The described coupling methods are numerically examined using two examples: uniaxial deformation and a plate with a hole relaxed under surface tension. Accuracy and convergence rates of each method are reported. A comparison to the solution as given by the surface-enchanced continuum is made [1,3]. It was found that the displacement (surface) coupling scheme and the Lagrangian (volume) scheme based on either discrete displacements or the H1 norm derived from continuous displacement fields provide the best performance. The financial support of the German Science Foundation (Deutsche Forschungsgemeinschaft, DFG), grant STE 544/46-1, and ERC Advanced Grant MOCOPOLY are gratefully acknowledged. 1. D. Davydov, A. Javili and P. Steinmann. On molecular statics and surface-enhanced continuum modeling of nano-structures. Computational Materials Science, Vol. 69, 510–519, 2013. 2. D. Davydov, J-P. Pelteret, P. Steinmann. Comparison of several staggered atomistic-to-continuum concurrent coupling strategies, Computer Methods in Applied Mechanics and Engineering, Vol. 277, 260-280, 2014. 3. D. Davydov, E. Voyiatzis, G. Chatzigeorgiou, S. Liu, P. Steinmann, M.C. Böhm, F. Müller-Plathe. Size effects in a silica-polystyrene nanocomposite: molecular dynamics and surface-enhanced continuum approaches, Soft Materials, Vol. 12, sup1, S142-S151, 2014.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Algorithms and High-Performance Computing for Hurricane Mitigation Analysis

Author(s): Clint Dawson, Jennifer Proft, Ali Samii, Wei Du, Gajanan Choudhary, *UT Austin*.

Hurricane and tsunami protection systems such as levees, gates, wetlands, etc. are being proposed for mitigation of surge along the coast. In this talk, we will focus on recent protection systems proposed for the Houston, TX region, and how probabilistic analysis is used to determine the efficacy of the proposed systems. The studies require advanced algorithms which capture multi-scale features of flow and coastal inundation, along with high resolution descriptions of the domain, bathymetry, topography, coastal inlets, and the various proposed protection systems. Flow through wetlands also complicates matters, and standard shallow water models may not be appropriate for these areas. We will discuss the Advanced Circulation (ADCIRC) modeling framework, and new physical and numerical models under development.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Numerical Assessment of Phase-Field Models for Fracture

Author(s): René de Borst, Stefan May, Julien Vignollet, *U. Glasgow*; Clemens Verhoosel, *Eindhoven U. Tech.*.

The modelling of cracks, including interfaces, is an important subject in the mechanics of materials. Basically, two methods exist to capture cracks. One possibility is to consider them as true discontinuities, i.e. in a discrete sense. Then, the mesh is adapted upon every change in the topology. Another approach is to model fracture within the framework of continuum mechanics. A fundamental problem then emerges, namely that standard continuum models do not furnish a non-zero length scale which is indispensable for describing fracture. To remedy this deficiency, regularization strategies have been proposed. The effect of these enrichments is that the discontinuity is transformed into a continuous displacement distribution. Gradient enrichments are among the most versatile among the regularization strategies. Interestingly, phase-field models for fracture, which recently have become en vogue, are closely related to gradient damage models. However, the point of departure is completely different. The basic idea in phase-field models is to replace the zero-width discontinuity by a small, but finite zone with sharp gradients in a mathematically consistent manner. Indeed, the latter requirement inevitably leads to spatial derivatives in the energy functional, similar to gradient damage models. In this contribution we will first review some basic concepts in brittle and cohesive fracture, and in phase-field modelling. Next, we will assess the performance of some recently proposed brittle phase-field models at the hand of elementary and established examples. We will investigate a number of factors that can critically affect the performance of phase-field models in brittle fracture, and also investigate the convergence of the smeared crack length with respect to the discrete crack length upon mesh refinement. Models for brittle and cohesive fracture rely on very different concepts, and the development of a cohesive phase-field model is a non-trivial task. A contribution on how to apply phase-field models to propagating cohesive cracks follows next, accompanied by one-dimensional and two-dimensional examples.

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Title: Variational Approach to FFT-Based Homogenization of Non-Linear Materials

Author(s): Tom de Geus, Ron Peerlings, Marc Geers, *Eindhoven U. Tech.*; Jaroslav Vondrejc, *U. West Bohemia*; Jan Zeman, *Czech Tech'l. U.*.

Computational multi-scale analyses have sparkled a wealth of new insights into many fundamental processes. Often these analyses rely on unit cell computations that accurately describe the underlying scale, for example the microstructure in a mechanical analysis. To minimize the effect of the finite dimensions of the unit cell, it is common to assume the unit cell periodic. In this paper, this assumption is employed to obtain an efficient numerical solution scheme. The success of the computational model often relies on the size of the considered unit cell (i.e. the allowed microstructural complexity) and the computational speed. For a mechanical analysis it was recognized by Moulinec and Suquet [1] that much gain on both aspects can be achieved by applying the discrete Fourier transform. Their approach, later generalized by Lebensohn and Roters [2] and others, resulted in a scheme that is both relatively simple to implement but most importantly computational efficient both in terms of memory and speed. The Moulinec and Suquet scheme uses the fundamental solution of an auxiliary problem to iterate towards mechanical equilibrium. For many non-linear problems such a fundamental solution does not exist, and frequently only an educated guess is used. In practice it is observed that this leads to slow convergence, or even failure to converge. In this paper, the mechanical equilibrium is solved using a weak formulation. The standard Galerkin scheme is applied, whereby the crucial ingredient is that Fourier polynomials are used for interpolation [3]. To this end the unit cell is discretized using a regular grid and each grid point is a numerical quadrature point. The crucial difference with the earlier scheme due to Moulinec and Suquet is that the resulting system is derived through linearization, and does not rely on a fundamental solution. It is shown that convergence is quadratic and unconditionally stable. It is noteworthy that the linearization on which this scheme relies is independent of the spatial discretization, interpolation, and quadrature so that the consistent tangent needs to be derived at the level of a material point. As a consequence, its implementation is irrespective of the choice interpolation and the same interface can be used for both FEM and FFT-methods. [1] Moulinec, H., Suquet, P., Comput. Methods Appl. Mech. Eng., 157(1-2):69-94, 1998. [2] Eisenlohr, P., Diehl, M., Lebensohn, R.A., and Roters, F. Int. J. of Plas., 46:37-53, 2013. [3] Vond\v{r}ejc, J., Zeman, J., Marek, I. Comput. Math. Appl., 68:151-73, 2014.

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Title: Geometric Discretization Through Primal-Dual Meshes

Author(s): Fernando de Goes, Mathieu Desbrun, *Caltech*.

This talk presents new computational tools for geometric discretization based on orthogonal primal-dual meshes. We start by introducing an optimal set of degrees of freedom for the construction of orthogonal primal-dual meshes on manifolds of arbitrary topology. We employ these reduced coordinates to reveal new properties on the duality between weighted triangulations and power diagrams, and also to extend these results to locally regular triangulations. By leveraging these structural properties, we derive effective discrete differential operators on primal-dual meshes and propose new algorithms for the generation of well-spaced polyhedral complexes and self-supporting triangulations. Finally, we exploit primal-dual meshes to design a new Lagrangian-based incompressible fluid solver that offers evenly-spaced particles over time and accurate pressure computations.

13th U.S. National Congress on Computational Mechanics
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Title: Condition Number Estimation and Improvement Strategies for the Isogeometric Finite Cell Method

Author(s): Frits de Prenter, Wing-Hin Wong, Clemens Verhoosel, Gertjan van Zwieten, Harald van Brummelen, *Eindhoven U. Tech.*.

Isogeometric analysis has been applied successfully to the discretisation of a variety of problems on geometrically and topologically complex volumetric domains by using it in conjunction with the finite cell method [Ruess,Schillinger,Harari]. In this method a structured, multivariate tensor-product domain is created in which the domain of interest is immersed. The trial and test spaces to be used in combination with a Galerkin problem are initially constructed over the structured domain, after which they are restricted to the domain of interest. Since an underlying structured mesh is available, local refinements can be obtained using hierarchical splines. A computational challenge posed by the finite cell method is that generally ill-conditioned systems are obtained [Ruess]. This ill-conditioning stems from the fact that some of the basis function supports only marginally intersect the domain of interest. In this contribution we study how the condition number of a finite cell system depends on the dimension and geometry of the domain of interest, the order of the differential equation, and the order of the basis functions. In this contribution we study two approaches for improving the conditioning of a finite cell system. In the first approach we employ a diagonal-like pre-conditioner. We show that the condition number can be improved drastically by appropriate scaling of the basis functions. In the second approach we employ local refinements to improve the conditioning of a system. We develop and study an algorithm that refines elements with small physical domain volume fractions. For both approaches we demonstrate the positive influence of the condition number improvement on conjugate-gradient solver performance. We present a comparison of the two studied approaches, and compare them to alternative pre-conditioning strategies available in literature. [Harari] A. Embar, J. Dolbow, and I. Harari. Imposing Dirichlet boundary conditions with Nitsche’s method and spline based finite elements. International Journal for Numerical Methods in Engineering, 83:877–898, 2010. [Ruess] M. Ruess, D. Schillinger, Y. Bazilevs, V. Varduhn, and E. Rank. Weakly enforced essential boundary conditions for NURBS-embedded and trimmed NURBS geometries on the basis of the finite cell method. International Journal for Numerical Methods in Engineering, 95:811–846, 2013. [Schillinger] D. Schillinger and M. Ruess. The Finite Cell Method: A Review in the Context of Higher-Order Structural Analysis of CAD and Image-Based Geometric Models. Archives of Computational Methods in Engineering, pages 1–65, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: Calibrating Model Errors in Multidisciplinary Analyses Using Time-Dependent Data

Author(s): Erin DeCarlo, Sankaran Mahadevan, *Vanderbilt U.*; Benjamin Smarslok, *Air Force Rsch. Lab.*.

Identifying and quantifying model errors in multidisciplinary analyses presents a unique calibration challenge due to the errors of one model being directly dependent the system state predicted by the previous analysis. In a time-marching scheme that executes two or more models in succession at each time step, all the model errors and uncertainty are further compounded across time steps. Limitations on experimental capabilities often prevent the complete replication of a coupled multi-physics response (e.g., fluid-thermal-structural interactions in a hypersonic flight environment), resulting in test data corresponding to a subset of the physics. Therefore, it is difficult to spatially and temporally isolate the input-dependent error contributions from each model using limited time-history data. The proposed methodology employs a Bayesian network approach using connections between models and available data to update parameters and quantify various sources of uncertainty: (1) natural variability in model inputs (e.g., materials and loading); (2) data uncertainty from measurement variability, experimental errors, and sparse data; (3) model errors due to simplified or poorly understood physics and numerical approximations. A model calibration framework developed by Kennedy and O'Hagan (KOH) represents each of these sources as nodes in the network. However, such developments in model calibration have only addressed single disciplinary analyses, or monolithic formulations of multidisciplinary analyses. The time-dependent Bayesian network used in this study has the ability to integrate information on any single discipline, or sets of disciplines, at any point in time during the simulation to gain insight on all uncertain nodes in the network, including parameters and errors in coupled disciplinary models. In this time-dependent Bayesian network approach, input-specific model errors are applied and calibrated incrementally at each time step. Appropriate error functions for transient coupled problems are particularly challenging because the errors are not a function of time, but rather a function of the current system state. Once suitable error models are determined for each physics-based model and applied incrementally at each time step, the contribution of each model's error can be identified across space and time, which enables model validation for the corresponding physics. The proposed error calibration approach will be demonstrated on transient aerothermal models within a coupled aerothermoelastic response prediction for structures subjected to extreme, combined, hypersonic environments. Time-dependent temperature data from wind tunnel experiments is used to quantify the predictive capabilities of the coupled aerodynamic heat flux and heat transfer models through spatial and temporal domains.

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Title: Computational Fluid Dynamics of the Heart: Coupled Models for Blood Flows in the Left Ventricle

Author(s): Luca Dede', Antonello Gerbi, Alfio Quarteroni, *EPFL*; Anna Tagliabue, *Politecnico di Milano, Italy*.

The simulation of the blood flow in the heart is a challenging task from both the mathematical and numerical points of view, mainly due to the different flow regimes developing during the heart beat, to the interaction with the valves, and, more in general, to the interaction of the heart components. In particular, the blood flow in the left ventricle depends on the mechanical contraction and relaxation of the muscle and on the interaction with the aortic and mitral valves, which mathematically define a complex fluid-structure interaction problem. In this respect, we focus on the computational fluid dynamics of the human left ventricle, with particular emphasis on the mathematical and numerical coupling with the dynamics of the heart valves and the muscle. Specifically, we show and discuss numerical results for the blood flows in idealized left ventricles, the interaction with the heart valves, and the coupling of the different components responsible for the heart functioning.

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Physics Analysis of Dry Storage Structures

Author(s): Masoud Dehghani Champiri, Arezou Attar, Mohammad Hanifehzadeh, Kaspar Willam, Bora Gencturk, *U. Houston*.

Abstract Normally dry storage casks are composite structures made of an inner steel liner and a concrete outerpack housing the basket of the spent nuclear fuel bundle. The main purpose of the cask structures is to provide safe storage of spent nuclear fuel elements exhibiting low levels of irradiation and temperature. Consequently, the upright storage cask structures are mainly subject to self-weight and environmental aging besides experiencing hazards of potential overturning in case of severe seismic events and man-made hazards. In this paper long-term performance of vertical dry cask structures are investigated and compared with their short-term behavior. Environmental aging is considered in the form of deleterious mismatch effects of steel and concrete creep on cask performance. The aging simulations include creep and shrinkage predictions of 1:3 scale cask models for 40 years of service using the B4 creep formulation of Bazant et al. [1] for concrete and the Bailey-Norton creep formulation for steel. The presentation will illustrate cask performance with the aid of COMSOL [2] predictions for hygro-thermal aging before the dry cask structure is subjected to tip-over contact-impact crash testing. The load scenario of the dry cask structures includes high temperature exposure of the inside steel liner, near the nuclear fuel basket, while the concrete outerpack is being held at a steady outside temperature. Self-weight, temperature gradient and environmental aging of the dry storage structure are considered in this paper before and during the final tip-over crash event. Elastic-perfectly plastic behavior of the steel liner and the three-invariant Willam-Warnke [3] formulation for concrete are used for the failure studies of the composite cask structure. The crash resilience of the composite cask structure is assessed using LSDYNA in order to quantify the effect of interface damage on the failure mode during tip-over crashing. The results of tip-over simulations of young concrete are compared with those of aged concrete considering the effect of accelerated environmental aging. References [1] Bazant, Z. P., Wender, R., Hubler, M. H. [2012], Report of RILEM committee TC-MDC, Multi-decade creep mpdel B4 for concrete creep and shrinkage including multi-decade prediction: description and application. [2] COMSOL Multiphysics®, The Platform for Physics-Based Modeling and Simulation, http://www.comsol.com/comsol-multiphysics. [3] Willam, K.J. and E.P. Warnke, (1974), “Constitutive Model for the Triaxial Behaviour of Concrete,” Proc. Intl. Assoc. Bridge Structl. Engrs, Report 19, Section III, Zurich, 1975, p. 30.

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Title: Surface Roughness Optimized Alignment of Parts for Additive Manufacturing Processes

Author(s): Patrick Delfs, Marcel Töws, Hans-Joachim Schmid, *U. Paderborn*.

All Additive Manufacturing (AM) processes have in common that they build up parts layer by layer. Unfortunately this layered structure results in a stair-stepping effect of the surface topographies. In general the impact of this effect strongly depends on the build angle of a surface, whereas the overall surface roughness is caused by the resolution of the specific AM process. The resolution in turn correlates to the used process parameter (e.g. layer thickness, tip size, energy rate of irradiation etc.) and material (e.g. melting viscosity, particle size distribution etc.). Other effects which influence the surface roughness are more process specific. The fused deposition modeling operates with the extrusion of polymer filaments with elliptic shape. The stacking of these filaments on a surface leads to a topography in build direction that looks like the magnitude of a sin function. In powder bed processes like polymer laser sintering incomplete molten particles stick on part surfaces and increase the surface roughness. Many AM processes need support structures to provide a base, stabilize overhangs and/or dissipate heat. The removal of these support structures from the part surfaces leave marks on the surface topography. As a consequence the topography of upward and downward directed surfaces can be different and the orientation in space has a big influence on the final surface quality (SQ) of a part. This leads to the ansatz of defining the build angle from 0° - 180° in respect to the building platform instead of reflecting all results by using only 0° - 90°. Aim of this work is the prediction of the SQ in dependence of the building orientation of a part. This results can finally be used to optimize the orientation to get a desired SQ. As explained above some surfaces won´t get well anyway, therefore it is possible in this model to indicate surfaces which don´t have to have a good SQ. The model uses the digital .stl format of a part as this is necessary for all AM machines to build it. Each triangle is assigned with a SQ value e.g. a roughness value and with testing different orientations the best one can be found. Of course this approach needs a dataset for the SQs. This must be done separately for each AM process and is shown exemplary with a surface topography simulation for the laser sintering process.

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Title: Parallel Collision Detection with WebCL for Web-Based Surgery Simulation

Author(s): Doga Demirel, Alexander Yu, Sinan Kockara, Tansel Halic, *U. Central Arkansas*.

This study presents a novel real-time collision detection algorithm using WebCL for interactive based surgery simulations on the web. The algorithm is based on a soft kinetic data structure called Dynamic Proximity Hierarchy (DPH) designed for both deformable and static body interactions for WebGL applications. WebGL, a 3D visualization technology in web browsers, becomes more embraced by graphics community due to its portability, backward/forward compatibility, and accessibility. However, WebGL based web applications experience performance bottlenecks due to interpreted execution. Although significant improvements have been made to speed up the execution time over the years with Just-In-Time compilers or recent high performance libraries such as Firefox asm [1], the performance drawback is still a major constraint. This becomes more acute in real-time WebGL applications such as surgery simulation allowing various user interaction modalities [2]. In such applications, collision detection is critical and computational expensive task that necessitates real-time execution rates. Especially in surgery simulation scenarios where deformable body collisions are common, achieving real-time execution rates is very challenging due to excessive topology-update operations. In this study, we design and develop a WebCL based DPH algorithm aims at increasing the speed up of collision detection execution with parallel execution. WebCL is a recently introduced technology allows JavaScript binding to OpenCL for heterogeneous parallel computing. Our WebCL based DPH algorithm overcomes performance bottleneck with harnessing parallel computing capability of the client device. We achieved real-time rates for complex virtual scenes composed of high resolution geometries. We present performance benchmarks with deformable and non-deformable body interactions in a virtual surgical scene to verify the execution speed-ups with respect to the serial DPH algorithm. We also tested our algorithm on various hardware devices to evaluate the scalability of the algorithm. References [1] “asm.js.” [Online]. Available: http://asmjs.org/. [Accessed: 15-Sep-2014]. [2] T. Halic, W. Ahn, and S. De, “A framework for web browser-based medical simulation using WebGL,” Stud. Health Technol. Inform., vol. 173, pp. 149–155, 2012.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Brittle Intergranular Fracture Frustrated by Intermittent Dislocation Emission

Author(s): Guoqiang Xu, Michael Demkowicz, *MIT* .

We investigated intergranular crack propagation in nickel using large-scale, fully 3-D molecular dynamics simulations. The crack front in our simulations is not parallel to any slip plane and is found to propagate in bursts in a brittle-like manner. Each burst begins with bond breaking and ends with copious dislocation emission. The crack tip is not fully blunted by the dislocations and remains sharp as it propagates. This counter-intuitive behavior occurs because the time-dependent stress intensity factory (SIF) continues to increase after onset of brittle crack propagation, even though the external load drops. The elevated SIF leads to the nucleation of dislocations, which in turn decreases the SIF and causes the crack to arrest. This is an important finding because it shows that, in contrast to the view espoused by the Rice-Thomson criterion, bond breaking and dislocation emission are not mutually exclusive. On the contrary, even in a nominally ductile material such as nickel, intergranular crack propagation is brittle at the atomic level. The effect of emitted dislocations is to prevent the brittle crack from propagating more than a few nanometers in a single burst. This work was supported by the BP-MIT Materials and Corrosion Center.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Discontinuous Petrov Galerkin (DPG) Method with Optimal Test Functions: A New Perspective

Author(s): Leszek Demkowicz, *UT Austin*.

The original idea of optimal test functions computed on the fly was coined within the framework of the ultraweak variational formulation [1]. Two years later [2] we learned that we could use the paradigm of broken test spaces and optimal test functions starting with the classical variational formulation. And only last year [3] we realized that the paradigm of ``breaking test functions'' can be applied to any well-posed variational problem. I will use the diffusion-convection-reaction model problem to review four possible variational formulations [4]: the trivial(strong) formulation, the classical one (analogue of Principle of Virtual Work for elasticity), the mixed method, and the ultraweak variational formulation. I will show then how each of these four variational formulations can be used as a starting point for applying the concept of optimal testing. The discussion will be illustrated with 2D numerical experiments. [1] L. Demkowicz and J. Gopalakrishnan. ``A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions. Numer. Meth. Part. D. E., 27:70--105, 2011. [2] L. Demkowicz and J. Gopalakrishnan. ``A primal DPG method without a first order reformulation.'' Comput. Math. Appl., 66(6):1058--1064, 2013. [3] C. Carstensen, L. Demkowicz and J. Gopalakrishnan, `` The paradigm of broken test functions in DPG discretizations'', in preparation. [4] L. Demkowicz. ``Various variational formulations and Closed Range Theorem,'', ICES Report 15-03.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: An Approach to Peridynamic Theory for Fractal Media

Author(s): Paul Demmie, *Sandia Nat'l. Lab.*; Martin Ostoja-Starzewski, *U. Illinois Urbana-Champaign*.

Fractal media are heterogeneous materials that exhibit fractal features over many length scales. Many natural and man-made objects approximate fractals to a degree, including coastlines, porous media, cracks, turbulent flows, clouds, rocks, soils, lightning bolts, brains, snowflakes, polymers, and biological materials. Since heterogeneities play a role over many length scales, traditional homogenization does not apply to such materials, and a consistent theory of deformation and failure of these materials under loading would be useful. Peridynamic theory is a theory of continuum mechanics that is formulated in terms of integro-differential equations without spatial derivatives. Therefore, the equations of peridynamics remain valid regardless of fractures or other discontinuities that may emerge in a body due to loading. This theory is a consistent formulation of both material deformation and failure, and has been applied to predict fragmentation of materials under loading. This presentation introduces an approach to peridynamic theory for fractal media. We review the modeling of fractal media by continuum mechanics using the method of dimensional regularization. The basis of this method is to express the balance laws for fractal media in terms of fractional integrals and, then, convert them to integer-order integrals in conventional Euclidean space. Following an account of this method, we discuss balance laws of fractal media, and propose an extension of these balance laws to the equations of peridynamic theory.

13th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Analysis of High-Cycle Fatigue and Damage Prediction Full Scale-Large Wind Turbines Including 3D Fluid-Structure Interaction

Author(s): Xiaowei Deng, Artem Korobenko, Jinhui Yan, Yuri Bazilevs, *UC San Diego*.

Wind turbines, converting mechanical energy to electricity, must extract as much wind energy from airflow as possible while resisting huge forces and deformations over a lifespan of 20 years. The size of wind turbine blade has been steadily increasing over the past few years with the limit of blade length expanding from 30~ 60 meters to 100 meters. However, large wind turbine may fail due to fatigue under millions of loading cycles over the long life span. Therefore we apply Paepagem's damage accumulation approach to simulate fatigue of composite blade. Wind turbine structure is modeled with Kirchhoff shell using isogeometric analysis. The aerodynamics is computed using a low-order finite element based ALE-VMS technique (ALE-based variational multiscale simulation). The enforcement of weak boundary conditions combined with track of non-matching meshes has been applied to the problem of wind and turbine interaction. The CX-100 wind turbine blade, developed by Sandia National Lab (SNL), is an experimental rotor design that includes a carbon fiber spar cap with a fiberglass shell laid over a balsa wood frame. Finally, our method is validated by the high-cycle fatigue simulation of the composite CX-100 rotor blades along with the complete path of damage progression including wind-turbine structure interaction. Future research can expand to the optimization of turbine blade design based on high-cycle fatigue simulation to extend its total fatigue life.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Parametric Study of the Dynamic Propagation of Offset Cracks Using the Phase-Field Method

Author(s): Sai Deogekar, Kumar Vemaganti, *U. Cincinnati*.

The study of the propagation of multiple cracks is critical to assessing structural reliability. The interaction between two cracks depends on a number of factors such as the domain geometry, the relative crack sizes and the separation between the two crack tips, and it affects the crack path of both the cracks. In this talk, we study the interaction between two dynamically propagating cracks. We use the phase-field method to track the crack paths since this method can handle complex crack behavior such as crack branching without any ad hoc criteria for crack propagation. First, we simulate crack interaction under static loading and compare it with experimental results to validate the model and then we simulate crack interaction under dynamic loading. The results from our dynamic simulations indicate that, unlike crack interaction under quasi-static or fatigue loading, the presence of another crack does not accelerate crack propagation when dynamic loads are applied. However, some similarities in the crack topologies are observed for both quasi-static and dynamic loading.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Predictive Numerical Models for Non-Linear Dynamic Behavior of Elastomer Damping Devices

Author(s): Jean-François Deü, Benjamin Morin, Antoine Legay, Lucie Rouleau, *CNAM*.

Due to their damping properties, elastomer materials are commonly used in the industry to achieve anti-vibration junctions between mechanical subsystems. These links are usually made of various materials (metallic, composites and elastomers) and have complex geometries based on the targeted application. In order to predict the dynamic behavior of these junctions in their environment, efficient numerical dynamic models must be developed. They should take into account the viscoelastic behavior of the elastomer and the material and geometric nonlinearity. The objective of this work is thus to develop effective models of flexible damping devices made of elastomer for the prediction of the dynamic behavior of complex systems. Firstly, a three-dimensional finite element nonlinear code using hyper-viscoelasticity constitutive relations is developed. Secondly, the parameters of the viscoelastic law are identified in the frequency domain from experimental tests using DMA (Dynamic Mechanical Analysis) [1]. This model is then transformed into an appropriate time-domain model in order to perform implicit dynamic simulations [2]. Finally, a reduced order model is developed. In linear dynamics, classical approaches are based on modal projection techniques which are adapted to highly damped structures. In nonlinear dynamics, this kind of methods can be extended using non-linear modes or proper orthogonal decomposition techniques. We propose in this study to construct models based on input-output laws connecting the generalized quantities of the faces of the junction in contact with substructures. In other words, the model links displacements and rotations of the faces to forces and torques applied to these faces. Moreover, due to the high number of parameters such as the direction, the amplitude or the frequency of the load, interpolation techniques are implemented to construct design response functions. [1] L. Rouleau, J.-F. Deü, A. Legay, F. Le Lay, Application of Kramers-Kronig relations to time-temperature superposition for viscoelastic materials, Mechanics of Materials, 65, 66-75, 2013. [2] J.-F. Deü, D. Matignon, Simulation of fractionally damped mechanical systems by means of a Newmark-diffusive scheme, Computers & Mathematics with Applications, 59 (5), 1745-1753, 2010.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Gauge Fixing Procedure for Spherical Lipid Vesicles

Author(s): Sanjay Dharmavaram, *UCLA*.

Lipid vesicles are observed to be area preserving fluid shells and are commonly modeled via the Helfrich energy. From a mathematical standpoint membrane fluidity manifests as reparametrization-invariance of the energy -- i.e., the energy is unchanged by arbitrary coordinate transformations of the reference state. It is well known that this symmetry leads to a redundancy in the Euler-Lagrange equations, wherein there are fewer equilibrium equations than degrees of freedom needed to determine the shape of the membrane, which leads to a gross indeterminacy in the formulation. The situation is particularly challenging for computations where indeterminate degrees of freedom appear as distortions of the finite element mesh and the presence of spurious modes. In this work we propose a procedure to remove the redundancy inherent to the problem and thereby make the system more amenable to effective computations. Borrowing terminology form physics, reparametrization-invariance, noted above, can be interpreted as a gauge symmetry. Breaking this symmetry, typically done by constraining the system with extra conditions(the so-called ``gauge-fixing procedure''), is tantamount to suppressing the redundant degrees of freedom of the system. In this work we propose a gauge-fixing procedure for spherical lipid vesicles which is achieved by supplementing the Euler-Lagrange equations of the Helfrich energy with the harmonic map equation (and a few subsidiary conditions). We show that this new augmented system completely breaks the reparametrization symmetry and consequently suppresses all the redundant degrees of freedom. Using a finite element formulation for this augmented system, we further demonstrate that the problem of mesh distortions can be eliminated.

13th U.S. National Congress on Computational Mechanics
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Title: Diffusion-Deformation Theory for Amorphous Silicon Anodes: The Role of Plastic Deformation on Electrochemical Performance

Author(s): Claudio Di Leo, Elisha Rejovitzky, Lallit Anand, *MIT*.

Amorphous Silicon (a-Si) is a promising material for anodes in Li-ion batteries due to its increased capacity relative to the current generation of graphite-based anode materials. However, the intercalation of lithium into a-Si induces very large elastic-plastic deformations, including volume changes of approximately 300%. We have formulated and numerically implemented a fully-coupled diffusion-deformation theory, which accounts for transient diffusion of lithium and accompanying large elastic-plastic deformations. The material parameters in the theory have been calibrated to experiments of galvanostatic cycling of an a-Si thin-film anode deposited on a quartz substrate, which have been reported in the literature. We have applied our numerical simulation capability to model galvanostatic charging of hollow a-Si nanotubes whose exterior walls have been oxidized to prevent outward expansion; such anodes have been recently experimentally-realized in the literature. We show that the results from our numerical simulations are in good agreement with the the experimentally-measured voltage versus state-of-charge behavior at various charging rates (C-rates). Through our simulations, we have identified two major effects of plasticity on the electrochemical performance of a-Si anodes: - First, for a given voltage cut-off, plasticity enables lithiation of the anode to a higher state-of-charge. This is because plastic flow reduces the stresses generated in the material, and thus reduces the potential required to lithiate the material. - Second, plastic deformation accounts for a significant percentage of the energy dissipated during the cycling of the anode at low C-rates. Hence, plasticity can have either a beneficial effect, that is, a higher state-of-charge for a given voltage cut-off; or a detrimental effect, that is significant energy dissipation at low C-rates.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Benchmark Study of Mode I Crack Opening for Brittle Materials

Author(s): Patrick Diehl, Marc Alexander Schweitzer, *U. Bonn*; Robert Lipton, *Louisiana State U.* .

We present a study for Mode I crack opening with simple bond-based Peridynamics [1] and the so-called Softening Material Model described in [2]. In this case we focus on the velocity at the crack tip once the crack start moving. A lattice-based approach for theoretical studies of crack tip instabilities for brittle materials is presented in [3]. Applying this to simple bond-based Peridyanmics yields a “semi-analytic” solution for the velocity at the crack tip. We present how to obtain the model parameters in the Softening model from the classical elasticity theory and the compared the obtained velocities in the simulations for polymethylmethacrylat (PMMA) with the presented “semi-analytic” solution. As a benchmark for the Softening model with used the velocity obtained in experiments and the numerical results for the lattice-based approach from [3]. [1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics, Computer & Structures, 38, 1526-1535 (2005). [2] R. Lipton, Dynamic brittle fracture as a small horizon limit of unstable nonlocal dynamics, Proceedings of the Society of Engineering Science 51st Annual Technical Meeting, 2014 [3] J. Fineberg and M. Marder, Instability in Dynamic Fracture, Physics Reports, 313, 1-108 (1999)

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Material Remap Algorithms for High-Order Finite Element Arbitrary Lagrangian-Eulerian (ALE) Simulations

Author(s): Robert Anderson, Thomas Brunner, Veselin Dobrev, Tzanio Kolev, Robert Rieben, *LLNL*; Vladimir Tomov, .

Arbitrary Lagrangian-Eulerian (ALE) methods are the basis of many multi-physics simulation codes. Our group develops ALE algorithms based on high-order finite element discretizations using the so-called "Lagrange plus remap" approach. During the Lagrange phase of ALE, the computational mesh follows the physical motion which in the presence of large deformations (e.g. vortical flow) leads to unacceptable mesh quality degradation. In order to correct this issue, a remesh step is introduced followed by an interpolation (remap) step to transfer the physical fields from the old mesh to the new. In multi-material problems, this algorithm naturally leads to the introduction of mesh elements (zones) which contain multiple materials —- mixed zones, which require careful treatment during the Lagrangian and remap steps of the algorithm. In this talk we describe our approach to mixed zone representation based on high-order discontinuous material indicator functions and focus on the multi-material remap algorithms we developed. Our approach to the remap problem is based on an advection formulation where the transition from the old Lagrangian mesh to the new mesh is given as a deformation field evolving in pseudo-time between the two states. We discretize this problem using a high-order discontinuous Galerkin (DG) scheme which is applied to the material indicator functions (or indicators) as well as the other physical fields. An important property of the indicators, that we want to preserve during remap, is that they are non-negative and sum to one. To ensure this, we consider synchronized monotonicity treatment based on flux corrected transport/remap (FCT/FCR) algorithm. Such corrections represent modifications to the volume transferred from one zone to another, and have to be taken into account when other fields, e.g. density, are remapped. In addition, special care must be used when all material-specific fields are transported to a zone, where that material was not previously present, in order to avoid creating new extrema. We will present our approach to resolving these conservation and monotonicity requirements, based on synchronized FCT treatment, and illustrate it with various multi-material examples. LLNL-ABS-667242

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Level Subset Simulation for Rare Evident Estimation with Application to Uncertainty Quantification in Composite Performance with Random Defects

Author(s): Timothy Dodwell, Richard Butler, Tatiana Kim, Robert Scheichl, *U. Bath*; Raphael Haftka, Nam Ho, *U. Florida*.

For aerospace applications the quantity of interest is often taken to be the probability a design will fail below a safe load. Understandably, this probability is very small, but obtaining robust estimates for these rare events is very difficult since, by definition, a large number of samples are required to observe even a single case. Furthermore the uncertain parameter space is often very large, and the scale and complexity of simulations mean even a single realisation is prohibitively (computationally) expensive. Classical methods that construct surrogates (e.g. polynomial chaos, sparse interpolation) are not feasible, suffering both from the curse of dimensionality and from the fact the tails (rare events) of the distributions are often very poorly approximated. Standard Monte Carlo (MC) methods perform little better. They are notoriously slow to converge and a large number of simulations are required to even observe a single rare event. To achieve sufficiently small sampling errors with equally precise modelling fidelity, such methods quickly become computationally unfeasible even for small-scale applications. In this paper we combine two novel stochastic methods; the Multilevel Monte Carlo Method (MLMC) [1] and Subset simulation [2], to achieve robust and efficient rare event estimation in large dimensional uncertain parameter spaces. The MLMC method achieves huge computational speed-ups [3] by taking advantage of combining a hierarchy of model fidelities, so that only a handful of costly fine scale computations are needed to accurately estimate probabilities. This work exploits this multilevel framework, and uses ideas from subset simulation in which samples are not drawn at random but biased towards parametric regions that cause premature failure. We examine the performance of the method in estimating the rare event failure probabilities for a composite application. The model set up is a 3D stack of carbon fibre composite, with randomly distributed tow/resin gaps, but also includes natural material variability and uncertain failure criteria. The methodology is used to efficiently calculate B- basis criterion for our model problem. This industrial requirement ensures that the probability of failure is less than 10% with 95% confidence. Reference [1] Cliffe, Giles, Scheichl, and Teckentrup, Computing and Visualization in Science, 14 (2011)3-15. [2] Au and Beck, Probabilistic Engineering Mechanics 16 (2001), 263 – 277. [3] Butler, Dodwell, T Kim, Kynaston, Scheichl, Haftka and N Kim, SciTech 2015, Kissimmee, Florida, 2015.

13th U.S. National Congress on Computational Mechanics
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Title: Incompressible N-Phase Flows: Physical Formulation and Numerical Algorithm

Author(s): Suchuan Dong, *Purdue U.*.

This work focuses on simulating the motion of a mixture of N (N>=2) immiscible incompressible fluids with given densities, dynamic viscosities and pairwise surface tensions. We present an N-phase formulation within the phase field framework that is thermodynamically consistent, in the sense that the formulation satisfies the conservations of mass/momentum, the second law of thermodynamics and Galilean invariance. In addition, we also present an efficient algorithm for numerically simulating the N-phase system. The algorithm has overcome the issues caused by the variable coefficient matrices associated with the variable mixture density/viscosity and the couplings among the (N-1) phase field variables and the flow variables. We compare simulation results with the Langmuir-de Gennes theory to demonstrate that our method produces physically accurate results for multiple fluid phases. Numerical experiments will be presented for several problems involving multiple fluid phases, large density contrasts and large viscosity contrasts to demonstrate the capabilities of the method for studying the interactions among multiple types of fluid interfaces. Reference: S. Dong, "An Efficient Algorithm for Incompressible N-Phase Flows", Journal of Computational Physics, 276, 691-728, 2014.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Random Sampling Strategies for Sparse Polynomial Chaos Expansions

Author(s): Alireza Doostan, Jerrad Hampton, *U. Colorado-Boulder*.

Sampling orthogonal polynomial bases via Monte Carlo is of interest for uncertainty quantification of models with high-dimensional random inputs, using Polynomial Chaos expansions. It is known that bounding a probabilistic parameter, referred to as coherence, yields a bound on the number of samples necessary to identify coefficients in a sparse PC expansion via solution to an L1-minimization problem. Utilizing asymptotic results for orthogonal polynomials, we bound the coherence parameter for polynomials of Hermite and Legendre type under the respective natural sampling distribution. In both polynomial bases we identify an importance sampling distribution, which yields a bound with weaker dependence on the order of the approximation. For more general orthonormal bases, we propose the coherence-optimal sampling: a Markov Chain Monte Carlo sampling, which directly uses the basis functions under consideration to achieve a statistical optimality among all sampling schemes with identical support. We demonstrate these different sampling strategies numerically in both high-order and high-dimensional expansions on several test problems.

13th U.S. National Congress on Computational Mechanics
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Title: Hybrid Collocation-Galerkin Approach for the Analysis of Surface Represented Solids

Author(s): Lin Chen, Sven Klinkel, *RWTH Aachen U.*; Wolfgang Dornisch , *Kaiserslautern U. Tech.*.

The paper presents a numerical method to solve the three-dimensional problem of surface represented solids. A boundary oriented element formulation is derived, in which the three-dimensional solid is described by its boundary surfaces and a radial scaling center. Scaling the boundary surfaces with respect to the scaling center describes the solids [1]. It conforms with the boundary representation modeling technique adopted in CAD. In the analysis, only the boundary surfaces of the solid will be discretized. No tensor-product structure of three-dimensional objects is exploited to parameterize the physical domain. Then, applying the weak form only on the boundary surfaces, the governing partial differential equations of elasticity are transformed to an ordinary differential equation (ODE) of Euler type. Solving the ODE leads to the displacement in the radial scaling direction. In the numerical implementation, the isogeometric Galerkin approach is employed to describe the boundary surfaces. It exploits the two-dimensional NURBS objects to parameterize the boundary surfaces. To solve the final Euler type ODE, the NURBS based collocation approach is applied [2]. Here, the higher continuity provided by NURBS allows to use collocation of the strong form of ODE instead of using the Galerkin method for the weak form. Collocation is applied between the center and the boundary. Thus, only one-dimensional collocation is used. Numerical integration is used only for the surface integrals at the boundary. Finally a set of equations is observed, where the number of equations is associated with the total number of collocation points. After considering the Dirichlet boundary conditions the reduced system of equations is solved for the unknown displacements. If a certain set of collocation points is used, the method is numerically stable [3]. The accuracy of the method is validated against the analytical solutions. In general, the proposed formulation will allow to model solids bounded by arbitrary number of boundary surfaces. References [1] C. Song, J. P. Wolf, The scaled boundary finite-element method-alias consistent infinitesimal finite-element cell method-for elastodynamics, Comput. Methods Appl. Mech. Engrg. 147 (1997) 329–355. [2] S. Klinkel, L. Chen, W. Dornisch, A NURBS based hybrid collocation-Galerkin method for the analysis of boundary represented solids, Comput. Meth. Appl. Mech. Engrg. 284 (2015) 689–711. [3] F. Auricchio, L. Beirão da Veiga, T. Hughes, A. Reali, G. Sangalli, Isogeometric collocation for elastostatics and explicit dynamics, Comput. Methods Appl. Mech. Engrg. 249-252 (2012) 2–14.

13th U.S. National Congress on Computational Mechanics
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Title: Patch-Coupling with the Mortar Method in Isogeometric Reissner–Mindlin Shell Analysis

Author(s): Wolfgang Dornisch, Ralf Müller, *U. Kaiserslautern*; Sven Klinkel, *RWTH Aachen U.*.

The novel idea of isogeometric analysis is to use the basis functions of the geometry description of the design model also for the analysis. Thus, the geometry is represented exactly on element level, and a closer integration of design and analysis is possible. Thin-walled structures are usually described by NURBS surfaces in industrial design software. Hence, an efficient isogeometric shell formulation is required in order to avoid costly conversions to other geometry descriptions. The higher continuity provided by NURBS surfaces requires special efforts in the case of Reissner–Mindlin shell formulations. The tensor-product character of NURBS surfaces yields quadrilateral topologies, and at the same time averts local refinement. Thus, methods to compute non-conforming discretizations are required in order to compute complex geometries consisting of several NURBS surface patches. An isogeometric Reissner–Mindlin shell formulation for nonlinear computations of complex structures involving arbitrary curvature and kinks is presented. The shell body is described by a shell reference surface, which is defined by NURBS surfaces, and a director vector. The rotational concept interpolates the axial vector of the rotations in combination with a multiplicative rotational update. The director vector in the current configuration is computed by an orthogonal rotation using Rodrigues' tensor in every integration point. The proposed rotational concept ensures proper convergence behavior also for high orders of basis functions. In this contribution a mortar method for the coupling of NURBS shell elements is proposed. A relation between the degrees of freedom of the master and the slave patch is derived from the weak form of the equality of deformations along the interface. This relation is used to compute mortar basis functions in the slave patch which are associated with degrees of freedom in the master patch. Thus, the interface degrees of freedom vanish from the global system of equation and the patches are connected. The weak form of the equilibrium is not altered. Several benchmark examples show the applicability of the coupling method and compare it to conforming computations. The accuracy of the presented shell formulation is not impaired by the usage of non-conforming discretizations.

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Title: Prediction of the Effective Elastic Moduli of Porous Solids Using Stochastic Micromechanical Modeling

Author(s): Borys Drach, *New Mexico State U.*; Andrew Drach, *UT Austin*; Igor Tsukrov, *U. New Hampshire*.

There are a number of analytic solutions in the literature that can be utilized to find contributions of pores to effective properties of linear elastic solids. Most of these solutions, however, are applicable to 2D cases with regular pore shapes, e.g. circular, elliptical, quasi-polygonal etc. In the 3D case of a solid with pores of irregular shapes, effective properties are typically determined using one of two approaches based on finite element analysis (FEA): 1) direct numerical simulations of a representative volume element (RVE, e.g. [1]); 2) micromechanical modeling via single-inclusion approach (e.g. [2]). The former method is usually computationally expensive and heavily dependent on the choice of RVE; the latter may be prohibitively time consuming due to large numbers of the pores: the sample analyzed in this work contained around 10,000 individual voids in 1 cubic centimeter volume. Thus, one of the main reasons for considering statistical approaches is the ability to construct prediction models based on characteristics of pore shapes that can be obtained without the FEA simulations. Another reason is to determine the pore geometric parameters that are of the most significance for overall elastic response of the considered composite. In this work, statistical modeling is used to correlate geometric parameters of pores with their contributions to the overall Young's moduli of linearly elastic porous solids. The proposed model is based on individual pore contribution parameters evaluated by FEA from a small subset selected using the design of experiments approach. A polynomial relating pore geometric parameters to the contribution parameters is fitted to the results of the simulations. It is shown that the accuracy of the model predictions depends on the choice of the pore geometry parameters as model factors. Our model is illustrated by considering a sample of carbon/carbon composite manufactured by chemical vapor infiltration of carbon fiber preform. This manufacturing process results in a porous material with highly irregular pore shapes. We found a good correlation between normalized projected areas of the pores on three coordinate planes and their contributions to corresponding effective Young's moduli. The results are compared with direct FEA simulations of computer generated periodic RVEs containing multiple pores. [1] Roberts, A.P., Garboczi, E.J., 2000. Elastic properties of model porous ceramics. J. Am. Ceram. Soc. 83
[2] Drach, B. et al., 2011. Numerical modeling of carbon/carbon composites with nanotextured matrix and 3D pores of irregular shapes. Int. J. Solids Struct. 48

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Title: Image-to-Mesh Conversion for Arteriovenous Malformation Surgical Simulators

Author(s): Fotis Drakopoulos, Nikos Chrisochoides, *CRTC Lab, Old Dominion U.*; Ricardo Ortiz, *KItware Inc.*; Andient Enquobahrie, *Kitware Inc.*.

In this paper we present our effort to build a push button Image-to-Mesh conversion software for blood vessels pertinent to Arteriovenous Malformations (AVM). AVMs are tangled bundles of abnormal vessels. Cerebral AVMs pose a threat of hemorrhage that could cause severe morbidity or death. Due to the risk and complexity of AVM surgery, neurosurgeons need to be highly trained. A realistic simulator will significantly improve the training process of allowing surgeons to have hands-on experience without jeopardizing patients health. However, interactive surgery simulation has made few inroads in neurosurgery due to many challenges. One of those challenges is insufficiently descriptive anatomic modeling (i.e., mesh generation) of the brain and particularly critical tissues such as blood vessels. First, we will describe the requirements analysis for AVM simulations and then the extensions of an existing general purpose mesh generation method we developed [1], for deformable registration of brain images from tumor resection using image guided neurosurgery. Our approach is based on a two-step procedure: (1) the creation of a Body-Centered Cubic (BCC) which creates a uniform structured BCC lattice and (2) the Mesh Compression step is used to smooth the BCC mesh in order to match the tissue(s) boundary. The BCC lattice is refined according to local feature size of labels in the 3D segmented image. The resolution of each tissue is automatically adjusted based on the user-defined fidelity (0, 1]. We will conclude with preliminary results and a comparison using: (i) a similar open source mesh generation method [2] and (ii) a Delaunay-based method [3], for general purpose image-to-mesh conversion. Our preliminary results indicate that we can achieve high fidelity, good gradation and quality of the elements. However, there is a trade-off between fidelity, gradation and element quality which needs to be studied in the context of Finite Element and collisions detection computations for AVM simulations --we plan to address next. [1] Multi-tissue mesh generation for brain images. Y. Liu, P. Foteinos, A. Chernikov and N. Chrisochoides. In 19th International Meshing Roundtable, pp 367-384, 2010. [2] Lattice Cleaving: Conforming Tetrahedral Meshes of Multi-material Domains with Bounded Quality. J. Bronson, J. Levine, R. Whitaker, In 21st International Meshing Roundtable, pp 191-207, 2012. [3] High Quality Real-Time Image-to-Mesh Conversion for Finite Element Simulations P. Foteinos and N. Chrisochoides. In Journal on Parallel and Distributed Computing, Vol. 74, No. 2, pp 2123-2140, 2014.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Hybrid Higher-Order Numerical Scheme for Convection-Diffusion Problems on Generic Grids

Author(s): Daniele Di Pietro, *U. Montpellier* ; Jerome Droniou, *Monash U.*; Alexandre Ern, *U. Paris-Est*.

Convection-diffusion equations permeate a variety of fluid flows models, including in particular flows in porous media. In such models, the natural diffusion can be in some places much smaller than the convection driven by the Darcy velocity, and it is therefore essential to dispose of numerical methods that can automatically and locally adapt to the flow regime (diffusion- or convection-dominated). Some practical constraints must also be taken into account, such as e.g. the capacity for the method to be efficiently implemented in a parallel environment. In this talk, we will present a numerical scheme of arbitrary order to deal with convection-diffusion equations. This scheme uses separate degrees of freedom on cells and faces, and has a local connectivity (each cell is only connected to its faces) which makes it a good candidate for parallel implementations. The discretisation of the convective terms uses a stabilisation which automatically adjusts to all regimes (including vanishing viscosity). This enables us to establish error estimates that are optimal in any regime, thanks to the usage of local Péclet numbers. References: 1. D. A. Di Pietro, J. Droniou, and A. Ern. "A discontinuous-skeletal method for advection-diffusion-reaction on general meshes". Submitted. http://arxiv.org/abs/1411.0098 2. D. A. Di Pietro, A. Ern, and S. Lemaire. "An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators". Comput. Meth. Appl. Math., 14(4):461–472, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: How Should Optimal 3D Tetrahedra be Defined and Constructed?

Author(s): Qiang Du, *Columbia U.*.

Mesh optimization is often related to finding the optimal element shapes having simple representation and providing good approximations. While regular triangles can be argued to optimal in 2D, the candidates for 3D optimal tetrahedra are up for debate. Meanwhile, 2D triangles are always subdivision invariant, the same does not always hold for their 3D counterparts. We present several interesting properties of 3D tetrahedra which are subdivision invariant and offer them a new classification. By studying the optimization of these tetrahedra, we argue that the second Sommerville tetrahedra are the closest to being regular and are optimal by many measures. Such tetrahedra also form the dual triangulation of the optimal 3D centroidal Voronoi tessellations. Anisotropic subdivision invariant tetrahedra with high aspect ratios are characterized. Potential implications to 3D unstructured tetrahedral meshing and applications of our findings are also discussed.

13th U.S. National Congress on Computational Mechanics
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Title: Some Nodal-Continuous Elements for Solving Non H1 Space Very Weak Solutions of Stokes Equations and Maxwell Equations

Author(s): Huoyuan Duan, *Wuhan U.*.

Stokes equations, in terms of velocity and pressure, with pressure Dirichlet boundary conditions while the velocity boundary condition is tangential, like Maxwell equations, may possess a non H1 space very weak solution. In the non-slip velocity boundary condition, the non H1 space very weak solutions would also exist. The well-known example is the so-called lid-driven cavity flow in which the velocity is not in H1 space and the pressure is in Lr for some r less than 2. Standard finite element methods with H1-conforming and nodal-continuous elements for both Stokes equations and Maxwell equations generally fail, with a wrong convergence. The so-called wrong convergence refers to the phenomenon that the finite element solution converges to an H1 solution, but not to the true solution which lies outside H1. In this talk, we consider a unified finite element method for both Stokes equations and Maxwell equations in two dimensions. We shall employ some well-known lower-order H1-conforming nodal-continuous elements for velocity and pressure. Satbility and convergence are analyzed. These elements are theoretically and numerically justified to correctly approximate the non H1 space very weak solutions. Meanwhile, the P1-P1 element and the classical and well-known P1 mini-P1 element are numerically shown to fail, resulting in wrong convergent finite element solutions. An example of the elements we shall consider is the well-known Taylor-Hood quadratic-linear element. We also consider some element for velocity which contains the gradient of a C1 element, such as HCT C1 triangle element. In general, the those non equal-order elements that are stable for the Stokes problem with velocity non-slip boundary condition are also stable and convergent for Maxwell equations and Stokes equations with pressure Dirichlet boundary condition.

13th U.S. National Congress on Computational Mechanics
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Title: Dynamic Fracture Characteristics of Metal Plate Under Blast Loading

Author(s): Yan Duan, Hui Lan Ren, Xiang Zhao Xu, *Beijing Inst. Tech.*.

The failure mode of the metal plate subjected to dynamic loads has been studied for many years[1], and most of the researchers concentrated on the response of plates instead of the fracture criterion. In this paper, the dynamic fracture characteristics of the plate under contact blast loading were explored by means of theoretical analysis and numerical simulation. On the basis of the damage evolution equation of metal and Cowper-Symonds material mode, a theoretical fracture criterion model to predict the fracture strain of the plate was proposed. According to the model, it is concluded that the fracture strain depends on the damage variables instead of the blasting loading. Besides, the paper presents the numerical work on the response of steel plates under explosion. In the numerical research, we put forward an improved method to overcome the limitation of the Eulerian method with fixed coordination by adding marked particles with influence domain into the parallel Eulerian computation program, pMMIC3D[2]. There are 4 kinds of relationship between the marked particle and the cell in which the particle is located, totally generating 27 cases. The particle value can be obtained from surrounding cells by weighted average. Based on the above improved method, a failure criteria about the effective strain was also added to the program for simulating the fracture process of the metal plate. Finally, the feasibility of the improved method was verified by comparing the results of the simulation and experiment, indicating that it could be used to simulate the failure of the metal plate subjected to blast loading. The numerical results under different working conditions, such as the fracture strain, exhibit the consistence with theoretical analysis. Reference: [1] V.H. Balden, G.N. Nurick, Numerical simulation of the post-failure motion of steel plates subjected to blast loading, International Journal Of Impact Engineering, 32 (2005) 14-34. [2] J.G. Ning, T.B. Ma, G.L. Fei, Multi-material Eulerian method and parallel computation for 3D explosion and impact problems, International Journal of Computational Methods,11 (2013) 1350079.

13th U.S. National Congress on Computational Mechanics
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Title: Consistent High-Order, Element-Free Galerkin Methods

Author(s): Qinglin Duan, Xin Gao, Bingbing Wang, Xikui Li, *Dalian U. Tech.* .

The element-free Galerkin (EFG) method invented by Belytschko et al. [1] is one of the major meshfree methods widely studied and used in the field of computational mechanics. One attractive advantage of this method is that constructing high order approximation is much more convenient than that in the finite element method (FEM). However, high order EFG is computationally inefficient since a large number of integration points are required. On the other hand, the stabilized conforming nodal integration [2] which proves very efficient for linear meshfree Galerkin methods cannot exploit the high convergence and the high accuracy of the EFG methods with high order approximation. In this work, the number of quadrature points for high order EFG is remarkably reduced by correcting the nodal derivatives. Such correction is rationally developed based on the Hu-Washizu three-field variational principle. The proposed method is able to exactly pass patch tests in a consistent manner and is therefore, named as consistent element-free Galerkin (CEFG) method [3]. In contrast, the traditional EFG cannot exactly pass patch tests. Numerical results show that the proposed CEFG method greatly improves the numerical performance of the high order EFG methods in terms of accuracy, convergence, efficiency and stability, especially the proposed cubic CEFG method which shows exceptional accuracy and convergence. In contrast, the cubic EFG method performs very poor in convergence and even worse, further increasing the number of quadrature points cannot evidently improve its numerical performance. This emphasizes the significance of the proposed technique for high order EFG methods. References: 1. Belytschko T, Lu YY, Gu L. Element-free Galerkin methods. International Journal for Numerical Methods in Engineering 1994; 37:229–256. 2. Chen JS, Wu CT, Yoon S, You Y. A stabilized conforming nodal integration for Galerkin mesh-free methods. International Journal for Numerical Methods in Engineering 2001; 50:435–466. 3. Duan QL, Gao X, Wang BB, etc. Consistent element-free Galerkin method. International Journal for Numerical Methods in Engineering 2014; 99:79–101.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Simulation of 3-D Hydraulic Fracture Propagation and Coalescence

Author(s): C. Armando Duarte, Piyush Gupta, *U. Illinois, Urbana-Champaign*.

Computational methods adopted in the oil and gas industry for the simulation of hydraulic fractures assume planar crack geometries. Several recent laboratory experiments and monitoring of actual field treatments however, suggest that a hydraulic fracture can grow in complex shapes due to local heterogeneities, layering, existence of natural fracture networks in the reservoir and interactions among hydraulic fractures. This presentation reports on recent advances of the Generalized Finite Element Method (GFEM) for three-dimensional hydraulic fractures. The proposed GFEM is able to handle (i) Simulations of 3-D non-planar fractures with complex geometries; (ii) Interaction and coalescence of 3-D non-planar crack surfaces and (iii) Simulations involving highly non-convex crack fronts. Discretization errors and computational cost are controlled through adaptive mesh refinement and enrichment. Strongly graded 3-D discretizations are automatically updated as the fracture evolves. Examples illustrating these features and the robustness of the method are presented.

13th U.S. National Congress on Computational Mechanics
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Title: The Finite Cell Method for Arbitrary Tetrahedral Meshes: Basic Principles

Author(s): Sascha Duczek, Ulrich Gabbert, *Otto-von-Guericke-U.* .

Keywords: Fictitious Domain Method, Finite Cell Method, Tetrahedral Finite Elements. The Finite Element Method (FEM) is the dominating numerical approach to solve Partial Differential Equations (PDE). It, however, suffers from the need for body-fitted discretizations. The mesh generation process can be viewed as the bottleneck in the simulation process, as it requires a lot of manual input and is rather error-prone. One idea to alleviate this drawback is to employ fictitious domain concept. Therefore, a simplified discretization using Cartesian grids is possible [1,2]. In combination with high-order shape functions the method is referred to as the Finite Cell Method (FCM) [1,2,3]. When geometrically complex industrial applications are in the focus of research activities it can be difficult to obtain a waterproof description of the surface of a component. Therefore, it may be hard to develop a suitable indicator function suitable for the numerical integration in the FCM framework. The main goal of the current paper is to retreat from the idea of using hexahedral cells and instead deploy tetrahedral ones. Thus, the finite element grids from commercial FEM pre-processors are transferred to the FCM and only important micro-structural details, such as pores etc. are included by deploying the principles known from the Fictitious Domain Concept (FDC). The geometry of the micro-structure is obtained by means of computed tomography (CT) where only the parts of interest are resolved with high resolution computer tomographs. The CT-scans can be either included into the FCM model by either using the voxelized data or by using surface tesselation language (STL) files to describe the boundary of the micro-structure. Accordingly, the influence of the micro level in regions of interest can be straightforwardly included in existing finite element models by means of the FDC applied to arbitrary tetrahedral discretizations. References [1] J. Parvizian, A. Düster and E. Rank. Finite Cell Method: h- and p-Extension for Embedded Domain Problems in Solid Mechanics, Computational Mechanics, Vol. 41, 121–131, 2007. [2] A. Düster, J. Parvizian, Z. Yang and E. Rank. The Finite Cell Method for Three-Dimensional Problems of Solid Mechanics, Computer Methods in Applied Mechanics and Engineering, Vol. 197, 3768–3782, 2008. [3] S. Duczek, M. Joulaian, A. Düster and U. Gabbert. Numerical Analysis of Lamb Waves Using the Finite and Spectral Cell Method, International Journal for Numerical Methods in Engineering, Vol. 99, 26–53, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: A Coupled Eulerian-Lagrangian Extended Finite Element Formulation for Simulating Morphology Evolution Due to Large Deformation of Hyperelastic Solids

Author(s): Ravindra Duddu, Anup Aryal, *Vanderbilt U.*; Louis Foucard, Franck Vernerey, *U. Colorado-Boulder*.

Many important and interesting problems in the areas of geophysics (e.g. ice sheet flow), soft material mechanics (e.g. swelling of hydrogels) and material science (e.g. metal forming) involve large to extreme deformation and mass flow. Purely Lagrangian finite strain formulations suffer from numerical issues due to excessive mesh distortion because the material is attached to the mesh nodes. The use of moving mesh techniques in conjunction with Lagrangian formulations (the Arbitrary Lagrangian-Eulerian formulation) could be cumbersome and still yield non-ideal meshes with large aspect ratio elements, eventually needing remeshing. On the other hand, Eulerian formulations that allow the material to move against the numerical mesh do not suffer from mesh distortion issues, however, specialized computational methods are required for modeling the evolution of domain boundaries or phase interfaces due to large deformation. In this presentation, a coupled Eulerian-Lagrangian (CEL) formulation aimed at modeling the moving interface of hyperelastic materials undergoing large to extreme deformations will be described. First, the model formulation based on the Eulerian description of kinematics of deformable bodies together with an updated Lagrangian formulation for the transport of the deformation gradient tensor will be discussed. Second, a mixed extended finite element and level set method used to discretize the equilibrium and transport equations in a two-phase medium will be described. Third, the grid based particle method used to evolve the level set function in order to capture the interface morphology evolution will be presented. Finally, the stability and accuracy of the computational method will be demonstrated through numerical benchmark simulations of compressible hyperelastic solids in two-dimensions.

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Title: From Fluid Mechanics to Magnetohydrodynamics: Challenges in the Finite-Element Modeling of MHD-Free Surface Flows

Author(s): Roland Rivard, *E. Polymtl.*; Steven Dufour, *E. Polymtl.* .

Since the eighties, the finite element community has overcome many challenges in order to successfully discretize the Navier-Stokes equations. Stable velocity-pressure element combinations, preconditioned iterative solvers, and turbulence models were in part responsible for this success. We now use these techniques on a regular basis for modeling a wide range of problems of fluid mechanics. The discretization of Maxwell's equations using the finite element method for the modeling of electrodynamics problems is a field that is not as mature. For example, studies using Nédélec elements (also known as edge elements in engineering) for modeling three-dimensional problems are still scarce, and effective preconditioning techniques still need to be found for these ill-conditioned discrete systems of equations. The numerical modeling of free surface flows has become increasingly important in computational fluid dynamics. Even if computational scientists have been proposing various strategies since the sixties, these problems are still difficult to model accurately. The fact that we are always studying more complex multiphysics problems does not make this task easier. We have been working for many years on the modeling of various free surface flow problems based on an interface capturing strategy. We recently have been involved in a project on the modeling of eddy-current problems, that led us to start exploring the modeling of magnetohydrodynamics free surface flows. These flows can be found, for example, in aluminum smelting cells. In this talk, we will share our recent experiences in modeling these complex multiphysics free surface flow problems, looking for inspiration in the work of the pioneers of the finite element method in fluid mechanics to overcome these new numerical modeling challenges. A novel numerical methodology for the modeling of large-scale magnetohydrodynamics free surface flow problems will be the end result of this research.

13th U.S. National Congress on Computational Mechanics
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Title: Mesoscopic Modeling of a Wire Strand for the Simulation of the Mechanical Behavior of Electrical Cables

Author(s): Baptiste Durand, Damien Durville, *MSSMat*; Guillaume Vega, *NRC Lens*.

Flexible electrical cables, specially used in aeronautics, are made of elementary wires arranged in two levels: they are first twisted to form so-called bunches, which are then stranded together. The study of the mechanical properties of these electrical cables requires the simulation of complexe structures made of few thousands of wires, too expensive to be conducted at this scale. We propose therefore a method to simulate these cables at the intermediate scale of bunches. The goal of our approach is to identify a mesoscopic model of bunch from simulations conducted at microscopic scale on a representative sample of bunch. Since wire trajectories within a bunch result from complex migration phenomena occurring during the twisting process, this process needs first to be simulated to get an initial configuration of a representative bunch sample. To do so we use a Finite Element code [1], based on an implicit solver, and focusing on the taking into account of contact-friction interactions within beam assemblies undergoing large transformations. Special boundary conditions allowing a proper rearrangement of wires at ends of the considered sample are used to simulate this initial twisting. Once the geometry of the reference bunch obtained, its response to various elementary loadings can be simulated, providing information at microscale related on the one hand to kinematics, and on the other hand to both elastic and dissipated (due to friction) energy. In order to build a mesoscopic model equivalent in energy to the test sample at microscopic scale, we proceed in two steps. First we propose an enriched beam kinematical model for the mesoscopic model of bunch, and identify projections of the kinematics at microscale on this intermediate kinematical model. Assuming an enriched beam kinematical model for the mesoscopic model, based on polynomials with respect to transverse coordinates, an appropriate projection will be used to express the kinematics identified at microscale in terms of the proposed beam kinematics. In order to derivate a mesoscopic constitutive law, relations between the strain computed form this mesoscopic kinematic and the mesoscopic energy will be sought. To do so, invariants with a physical significance [2] will be used. [1] D. Durville (2012). Contact-friction modeling within elastic beam assemblies: an application to knot tightening. Computational Mechanics, 49(6), 687-707. [2] J.C. Criscione, A.S. Douglas, & W.C. Hunter (2001). Physically based strain invariant set for materials exhibiting transversely isotropic behavior. Journal of the Mechanics and Physics of Solids, 49(4), 871-897.

13th U.S. National Congress on Computational Mechanics
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Title: Numerical Simulation of the Mechanical Behavior of Fibrous Materials at Microscopic Scale

Author(s): Damien Durville, *CNRS / CentraleSupelec*.

The mechanical behavior of fibrous materials and structures is highly dominated by contact-friction interactions taking place between their elementary components. A finite element approach, based on an implicit solver, and designed to solve the mechanical equilibrium of general beam assemblies, is proposed to simulate the mechanical behavior of such materials. This approach is based on the detection and modeling of contact-friction interactions occurring between fibers represented by finite strain beam elements. Since textile materials are often made of fibers arranged according to several nested levels (e.g. to form successively threads, yarns, and woven fabrics), special hierarchical boundary conditions are considered to allow sub-components of different levels to rearrange while satisfying average conditions formulated at each level. Fibrous material samples corresponding to various arrangement patterns (twisted yarns, braided ropes, 3D interlock woven fabrics) may be handled by this approach. As in most cases the initial configuration of such structures cannot be known a prior since it depends on manufacturing process, simulation is used first to determine the unknown initial geometry, starting from a simple arbitrary configuration, and letting contact interactions gradually separate fibers from different sub-components, according to the selected arrangement pattern. Determination of initial configurations of braided ropes and 3D interlock fabrics will be presented. The simulation of various loading allows macroscopic mechanical properties of such materials to be determined. Very useful information at microscopic scale is obtained from these simulations, especially in terms of heterogeneous stress distribution among constitutive fibers, helping to understand complex internal mechanisms. Durville, D. (2012). Contact-friction modeling within elastic beam assemblies: an application to knot tightening. Computational Mechanics, 49(6), 687-707. Vu, T. D., Durville, D., & Davies, P. (2015). Finite element simulation of the mechanical behaviour of synthetic braided ropes and validation on a tensile test. International Journal of Solids and Structures.

13th U.S. National Congress on Computational Mechanics
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Title: Massively Parallel-In-Space-Time, Adaptive Finite Element Framework for Non-Linear Parabolic Equations

Author(s): Robert Dyja, *Czestochowa U. Tech.*; Kris Van Der Zee, *Nottingham*; BASKAR GANAPATHYSUBRAMANIAN, *Iowa State U.*.

We present an adaptive methodology for the solution of (linear and) non-linear time dependent problems. The basic concept is to solve for large blocks of space-time unknowns instead of marching sequentially in time. The methodology is a combination of a computationally efficient implementation of a parallel-in-space-time finite element solver coupled with a posteriori space-time error estimates and a parallel mesh generator. This methodology enables simultaneous adaptivity in both space and time (within the block) domains. We explore this basic concept in the context of a variety of time-steppers including Θ-schemes and Backward Difference Formulas. We specifically illustrate this framework with applications involving linear, quasi-linear and non-linear diffusion equations. We focus on investigating how the coupled space-time refinement indicators for this class of problems affect spatial adaptivity. Finally, we show good scaling behavior up to 150,000 processors on the Blue Waters machine. This is achieved by interlacing time-domain degrees of freedom -- which provides memory locality, and careful usage of memory via block storage and non-zero formats along with lumped communication for matrix assembly. This methodology enables scaling on next generation multi-core machines by simultaneously solving for large number of time-steps, and reduces computational overhead by refining spatial blocks that can track localized features. This methodology also opens up the possibility of efficiently incorporating adjoint equations for error estimators and inverse design problems, since blocks of space-time are simultaneously solved and stored in memory.

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Title: VoroCrust Algorithm: 3D Polyhedral Meshing with True Voronoi Cells Conforming to Surface Samples

Author(s): Ahmed Mahmoud, *Alexandria U.*; Ahmad Rushdi, Chandrajit Bajaj, *UT Austin*; Scott Mitchell, Mohamed Ebeida, *Sandia Nat'l. Lab.*; John Owens, *UC Davis*.

We introduce VoroCrust for creating polyhedral meshes of 3D solids enclosed by 2D surfaces. VoroCrust is the first algorithm for 3D Voronoi meshes that naturally *conform* to sampled surface points. Conformality is distinguished from the usual *clipping* of Voronoi cells by the surface, which always results in extra surface vertices beyond the original samples, and may result in non-planar, non-convex, or even non-star-shaped cells. VoroCrust creates cell seeds such that points previously generated on the manifold are vertices of the 3D cells, and the only surface vertices. This avoids shrinkage and other changes. All cells are true Voronoi cells; the surface does not restrict or constrain the Voronoi cells, rather the cells are geometrically placed to reconstruct the surface, by the cell facets separating inside and outside seeds. These facets are well-shaped and usually triangles. Mesh polyhedra enjoy all the nice properties of Voronoi cells, such as being convex with planar facets. Cell aspect ratios and dihedral angles are bounded. We have not yet addressed the issues of small edges, sharp edge angles, and small area faces, which may be important for some types of simulations. In contrast to the well-known 'power crust' surface reconstruction algorithm, VoroCrust fills the volume with tunable 3D cells with good shape, that is, VoroCrust output is usable as a finite volume mesh. Also, VoroCrust's 2D manifold reconstruction is from an *unweighted* Voronoi diagram, which supports fast inside/outside queries. The VoroCrust algorithm starts by creating surface sample points. We use Poisson-disk Sampling (MPS), placing points densely compared to the local thinness and curvature, with additional algorithms for sharp and thin features. (Or the points may be generated by some other surface other triangulation mesher and given as input.) In either case we create spheres around samples. We define triple-intersection points as Voronoi seeds near the surface. We create additional seeds interior to the volume; we have algorithms to place these randomly, or in a structured way to create a hex-dominant mesh. We generate the 3D Voronoi tessellation of all these seeds. The manifold is reconstructed by the Voronoi facets separating the inside and outside cells. This talk describes the algorithmic and engineering aspects of VoroCrust, especially the surface sampling (meshing) and mesh grading. Scott Mitchell's talk in MS714 ('Voronoi Dual Meshing and Simulation') describes the geometric and theoretical aspects of generating the seeds from the surface sample spheres.

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Title: Peridynamics Analysis of Elastic-Plastic Contacts

Author(s): Sayna Ebrahimi, Kyriakos Komvopoulos, David Steigmann, *UC Berkeley*.

Peridynamics is a nonlocal method based on a continuum of particles in the neighborhood of a given particle [1,2]. The neighboring particles transmit forces to the given particle. This is represented by an integral summation of all the particle forces. In turn, these forces depend on the distance of the given particle relative to those in its predefined neighborhood. The governing equations in peridynamics are in integral form instead of differential form. This facilitates the modeling of material discontinuities, which need only to satisfy the requirement of integrability, rather than the significantly more stringent and restrictive requirement of differentiability of conventional methods. Peridynamics has been mostly applied to analyze various fracture mechanics problems (e.g., [3]). However, the capabilities of this theory can also be extended to many other problems in solid mechanics. In this study, a peridynamics framework is developed for elastic and elastic-plastic solid contacts. The focus is on accurately capturing contact behavior, in particular the evolution of contact pressure distribution, contact area, and subsurface stress and strain fields. Numerical results are compared with existing analytical solutions to validate the developed peridynamics approach. References: [1] Silling, Stewart A. "Reformulation of elasticity theory for discontinuities and long-range forces." Journal of the Mechanics and Physics of Solids 48.1 (2000): 175-209. [2] Silling, Stewart A., et al. "Peridynamic states and constitutive modeling." Journal of Elasticity 88.2 (2007): 151-184. [3] Silling, Stewart A., and Ebrahim Askari. "A meshfree method based on the peridynamic model of solid mechanics." Computers & structures 83.17 (2005): 1526-1535.

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Title: New Insights in Fatigue Crack Initiation and Small Crack Growth Regime: Coupled Micro-Mechanical Testing and Crystal Plasticity Modeling

Author(s): Panos Efthymiadis, Richard Dashwood, Barbara Shollock, *Warwick U.*; Christophe Pinna, *U. Sheffield*; John Yates, *Simuline Ltd.*.

The paper reports on part of our current research effort to understand the role of various microstructural features on Fatigue Crack Initiation (FCI) in metallic alloys. By employing a novel experimental set-up, in situ micro-mechanical testing was performed inside an SEM chamber, and the deformation of individual grains was observed in real time during a cyclic fatigue test. A 4-point bend specimen containing a machined hole of 1mm was used for both testing and modeling. A physically-based Crystal Plasticity (CP) model was built that simulates both the macro and micro mechanical behaviour of Al2024 T3, and a comparison was made between the simulated and experimental results. An experimentally informed FCI criterion was then developed that accounts for the effect of local slip bands and the applied local strains. Furthermore, new insights were acquired into the short crack growth regime by observing the micro-scale phenomena during the test and comparing with simulations using an XFEM technique. The approach developed has been applied in other aerospace alloys, such as nickel superalloys and advanced high strength steels.

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Title: Hydro-Mechanical Description of Saturated Fractured Porous Media Based on Microporomechanics

Author(s): Mahdad Eghbalian, Richard Wan, *U. Calgary*.

Hydraulic Fracturing is used in unconventional gas reservoirs, notably tight gas or shale gas reservoirs where the permeability is extremely low. As such, it is important to understand the process by which the material fails through fracture formation to increase flow, and hence production. At issue is the understanding of both physical and numerical aspects of fracture initiation and propagation in quasi-brittle materials, including multiphase flow. Various fracture regimes can be identified such as one which is diffuse (where fractures are tiny and ubiquitous) to an ultimate localized mode where certain micro-fractures coalesce into a macro-fracture. Conditions upon which the various fracture regimes occur as a function of loading (mechanical or fluid stimulation) type can be studied from the mechanics damage in a random heterogeneous quasi-brittle material. In this paper, the fracture behavior of cemented materials such as rock consisting of randomly distributed micro-cracks is addressed with coupled physics and in a Hydro-Mechanical (HM) framework. Homogenization technique is utilized to formulate a continuum description of such heterogeneous material based on observed microscopic physical mechanisms. A representative volume element (RVE) of the medium is considered at the meso-level, and by investigating a detailed description of the micro-structure, the average quantities over the whole RVE and the underlying relations between them (constitutive equations) are determined at the continuum level, considering both solid and fluid phases. Hence, coupled fluid flow and deformation mechanisms of homogeneous porous medium can be described based on the mechanical properties of solid and fluid phases at the micro-scale. The presence of heterogeneities in form of randomly distributed micro-cracks is addressed here by formulating a one-way coupled problem at the meso-scale. The macroscopic behavior is then described by the relation between relevant macro quantities through a homogenization scheme. An anisotropic damage model is developed to capture the reduction in load bearing capacity and permeability evolution of the porous medium to help us predict the fracture occurrence in the reservoir under general loading condition. The evolution of the damage is studied through fracture mechanics and by formulating the strain energy release rate to describe the stable growth of micro-cracks under general loading conditions. Keywords: Hydraulic Fracturing; Micro-cracks; Hydro-Mechanical; Homogenization; Damage model

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Title: Approximation of Effective Coefficients in Stochastic Homogenization Using a Boundary Integral Approach

Author(s): Virginie Ehrlacher, *Paris-Tech/INRIA*.

(joint work with Eric Cancès, Frédéric Legoll and Benjamin Stamm) A very efficient algorithm has recently been introduced in [1] in order to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies in the clever use of a boundary integral formulation of the problem to solve. The aim of this talk is to present how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this aim, the definition of new approximate corrector problems and approximate effective coefficients is needed and convergence results in teh spirit of [2] are proved for this new formulation. Some numerical test cases will illustrate the behaviour of this method. [1] "Domain decomposition for implicit solvation models", Eric Cancès, Yvon Maday, Benjamin Stamm, The Journal of Chemical Physics 139 (2013) 054111 [2] "Approximations of effective coefficients in stochastic homogenization", Alain Bourgeat, Andrey Piatnitski, Annales de l'institut Henri Poincaré (B) Probabilités et Statistiques 40 (2004) page 153-165

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Spatial and Temporal Coarse Graining in Dislocation Dynamics: Capturing the Elusive Cell Structure in Deformed Metals

Author(s): Anter El-Azab, *Purdue U.*.

In this contribution we describe a mathematical approach to the spatial and temporal coarse-graining of dislocation dynamics and the development of a continuum density based theory of dislocation dynamics. The coarse graining is based on the framework of statistical mechanics in the spirit of the classical kinetic theory, which leads to a hard closure problem consisting of finding the spatial and temporal correlations and determining such correlations from discrete dislocation dynamics. A novel approach was developed to determine the continuum rates of cross slip and annihilation reactions and incorporate those into the continuum framework stochastically. We prove the effectiveness of this framework by making the first known prediction of dislocation cell structure under monotonic loading of copper. This presentation consists of a short review of relevant models, a description of the mathematical framework of dislocation coarse-graining, and presenting a full solution of the problem using a novel finite element approach. This work was performed in collaboration with Jie Deng, Mamdouh Mohamed and Shengxu Xia.

13th U.S. National Congress on Computational Mechanics
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Title: Non-Equilibrium Thermodynamics of Fault Gouge: Effect of Grain Contact Processes

Author(s): Ahmed Elbanna, *UIUC*; Charles Lieou , Jean Carlson, *UCSB*.

Granular materials are ubiquitous in nature. They play an important role in the physics of many natural phenomena like earthquakes and landslides as well as many industrial applications such as in food and pharmaceutical industries. In this presentation we present our latest progress in developing a non equilibrium statistical thermodynamics framework for describing plasticity in amorphous materials such as the crushed rocks found in fault zone, commonly known as fault gouge. We show the in the limit of perfectly hard sphere, the material response is rate strengthening. The predicted shear strength exhibit weak rate dependence for low values of inertial number but it increases rapidly as the inertia number approaches a critical value nearly equal to 1. To reproduce rate weakening behavior, as well as non-monotonic rheology, observed in a variety of experiments additional theoretical components describing physical processes at the grain contacts must be introduced. We present a few candidates for these processes including flash heating at contact asperities and grain breakage. We discuss the implications of non-monotonic rate dependence on stability of frictional sliding and stick-slip motion.

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Title: Preconditioned MCMC and Adaptive Posterior Refinement Leveraging Sparse Polynomial Chaos

Author(s): Michael Eldred, John Jakeman, Laura Swiler, *Sandia Nat'l. Lab.*.

The process of performing Bayesian inference is frequently hindered by expense and by a lack of reliability in the Markov-Chain Monte Carlo (MCMC) sampling used for computing the posterior distribution. In this talk, we present an adaptive emulator-based inference algorithm that seeks to improve MCMC efficiency and reliability, while supporting moderate-to-high dimensionality through the use of sparse recovery of polynomial chaos coefficients. Starting from a sparse polynomial chaos emulator constructed over the support of the prior distributions using L1-regularized regression, we will employ analytic derivative information from the emulator to inform the proposal density to accelerate the MCMC process. For a given posterior estimate computed for the current emulator, we will then refine the emulator by performing new model evaluations for samples with high posterior density, as evaluated using either chain filtering or density estimation. Convergence in this adaptive refinement process will be determined using relative change in the posterior distribution, as evaluated using distribution distance metrics. The result is a more efficient and reliable inference component that will enable meta-inference processes such as Bayesian model selection.

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Title: Capturing the Role of Fiber Orientation in Drug-Induced Cardiac Electro-Mechano-Physiology

Author(s): Noha Shalabi, *American U. Cairo*; Nejib Zemzemi, *INRIA*; Khalil Elkhodary, *American U. Cairo*.

Precise drug intervention can control the chemical reactions evolving on nanoscale cellular structures. As a result the ionic currents, mainly soduim potassium and L-type Calcium, could be modified from their control conditions. In this case the electrical wave propagating in the heart tissue is modified which could alter the macroscale cardiac mechanical behavior. As such, a deeper understanding of the multiscale links between drug chemistry and cardiac electro-mechanics holds promise for new cures to various heart diseases. We herein advance a computational approach to further this understanding. We simulate the electrical activity of the heart based the state-of-the-art reaction-diffusion mono-domain model. We introduce the drug/ion channels interaction using a pore block model [1]. As concerns the mechanical model, we use an anisotropic hyperelastic material law for cardiac muscle tissue [2]. Fiber directions in cardiac muscle walls are generated on physiological grounds, based on the Streeter algorithm [3]. We have also added visco-elastic robin-like boundary condition in order to take into account the constraints applied by organs surrounding the heart. The resulting model is implemented in the open-source computational biology library CHASTE. Our simulations introduce different drugs and drug concentrations to the cellular model, and comparison is made against control values from literature and available medical imaging data, using global metrics, such as shortening in the base-to-apex direction, and local metrics, such as the Lagrangian circumferential strain as a measure of contraction. [1] Zemzemi et al., Computational assessment of drug–induced effects on the electrocardiogram: from ion channel block to body surface potentials, British Journal of Pharmacology, Vol. 168, No. 3, pp. 718–733, 2013 [2] Rossi et al., Orthotropic active strain models for the numerical simulation of cardiac biomechanics, International Journal for Numerical Methods in Biomedical Engineering, 2012 [3] Streeter et al., Fiber orientation in canine left ventricle during diastole and systole, Circulation Research, Vol. 24, pp. 339–47, 1969

13th U.S. National Congress on Computational Mechanics
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Title: SPH Simulation of Concentrated Suspensions Under Confinement

Author(s): Adolfo Vazquez Quesada, Marco Ellero, *Swansea U.*.

In this talk we will present a three-dimensional extension of a SPH-based particle model of concentrated suspensions already tested under confined two-dimensional flows in [1]. Solid suspended particles are modelled by using frozen boundary particles with artificial velocities assigned in order to satisfy no-slip boundary condition on the solid-liquid interface. As described in [2] for large particle concentrations, capturing accurately the dynamics of nearly contacting solid particles is a numerical challenge due to the singular short-range behavior of interparticle lubrication forces. In this talk we extend the semi-implicit splitting scheme presented in [2] by incorporating, beside normal interparticle lubrication, also tangential lubrication effects into a full three-dimensional system. The method is tested by comparing the overall suspension viscosity against established numerical results [3] and experimental data for non-colloidal suspensions in Newtonian media [4]. Unlike standard numerical approaches using Irving-Kirkwood theory applied to a bulk system, here the suspension is confined between parallel plates and viscosity is measured deriving it from real forces acting on the plates, in a similar fashion to experimental setups. Finally, effect of geometrical confinement on the measured suspension rheology will be discussed. [1] Hydrodynamic shear thickening of particulate suspension under confinement X Bian, S Litvinov, M Ellero, NJ Wagner, Journal of Non-Newtonian Fluid Mechanics 213, 39-49 (2014). [2] X. Bian, M. Ellero, "A splitting integration scheme for the SPH simulation of concentrated particle suspensions", Comp. Phys. Comm. 185, 5362 (2014). [3] E. Bertevas, X. Fan, R.I. Tanner, "Simulation of the rheological properties of suspensions of oblate spheroidal particles in a Newtonian fluid" Rheologica acta 49 (1), 53-73 (2010). [4] S.C. Dai, E. Bertevas, F.Z. Qi, R.I. Tanner, "Viscometric functions for noncolloidal sphere suspensions with Newtonian matrices", Journal of Rheology 57 (2), 493-510 (2013).

13th U.S. National Congress on Computational Mechanics
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Title: Space-Time Discontinuous Petrov-Galerkin Finite Elements for Fluid Flow

Author(s): Truman Ellis, Leszek Demkowicz, *UT Austin*; Jesse Chan, *Rice U.*; Nathan Roberts, *Argonne Nat'l. Lab.*.

The discontinuous Petrov-Galerkin method is a novel finite element framework with exceptional stability and adaptivity properties. The DPG framework can be used to derive stable discretizations of any well-posed variational formulation and has been successfully applied to problems such as heat conduction, time-harmonic Helmholtz, Maxwell's equations, linear elasticity and plate problems, Stokes flow, and both incompressible and compressible Navier-Stokes. In contrast to many other numerical methods, DPG does not suffer from a pre-asymptotic regime (unstable behavior on coarse meshes). This means that a simulation can be initiated at the coarsest scale possible while automatic adaptivity resolves solution features based on a robust, built-in measure of residual error. DPG is intensely locally compute intensive with significant embarrassingly parallel computations done both pre- and post-global solve. We present work on a space-time DPG formulation for fluid dynamics applications that enables automatic local time stepping and a kind of parallel-in-time integration.

13th U.S. National Congress on Computational Mechanics
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Title: Efficient, Multi-Scale Structural Reliability Predictions for Engineering Applications

Author(s): John Emery, Richard Field, Joseph Bishop, Jay Carroll, *Sandia Nat'l. Lab.*.

Prediction of structural failure due to strain localization or fracture is an essential engineering challenge where ultra-high reliability (e.g., failure probability <1e-06) is required. Heterogeneity at the fine scale can contribute to significant uncertainties in performance, particularly for small-scale components. Practical applications cannot include fine-scale details throughout the problem domain due to exorbitant computational demand. A concurrent multiscale numerical method is necessary but not sufficient. One multiscale calculation does not answer the question because there is no way to know if it represents the best-case scenario, the worst-case scenario or some average of scenarios. To illustrate, a multiscale finite element analysis coupling a polycrystalline subdomain to one hotspot in a component typically requires the solution to 100’s of millions of equations for one realization of the microstructure – a very computationally expensive endeavor. This represents only one data point for the conditional probability of failure assuming failure occurs at that hotspot. There are presumably many hotspots and many possible microstructural configurations. To complete a reliability assessment, Monte Carlo simulation (MCS) is necessary at each hotspot, requiring many thousands of such analyses – this is intractable. We propose a novel algorithm to efficiently perform MCS hierarchically across length scales employing stochastic reduced-order models. The algorithm starts with the engineering scale and produces a low-fidelity prediction that is refined with multiscale simulation. This talk will outline the proposed hierarchical solution scheme and present numerical studies for demonstration. (*Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.)

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Title: Topology Optimization with Local Stress Constraints: A Level Set with a Polygonal, Finite-Element Approach

Author(s): Helio Emmendoerfer Jr, *Fed'l. U. Santa Catarina; U. Illinois Urbana-Champaign*; Eduardo A Fancello, *Fed'l. U. Santa Catarina*; Glaucio H Paulino, *Georgia Inst. Tech.*.

This work focuses on topology optimization for mass minimization with local constraints on the von Mises stress field. We develop a procedure to account for continuous activation/deactivation of stress constraints. Such constraints are incorporated to the objective function by means of an augmented Lagrangian within the level set context. The level set evolution makes use of a reaction-diffusion equation and sensitivity analysis to update the structural topology. This level set technique allows the nucleation of holes and precludes the need for reinitialization. The numerical solution is accomplished by means of polygonal elements. Unstructured polygonal meshes provide greater flexibility in discretizing arbitrary (e.g. non-Cartesian) domains and attractive features to model microstructural details (e.g. inclusions). The features of this approach are demonstrated by a set of benchmark examples in two dimensions in order to assess the capability of the algorithm to identify stress concentrations that can lead to feasible designs and connect with additive manufacturing.

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Title: TriGA: Generalization of Isogeometric Analysis to Unstructured Triangular and Tetrahedral Discritizations

Author(s): Luke Engvall, John Evans, *U. Colorado-Boulder*.

Isogeometric analysis was introduced as a way to bypass the design-to- analysis bottleneck inherent in the traditional CAD through FEA paradigm. However, an outstanding problem in the field of IGA is that of surface-to-volume parameterization. In CAD packages, solid objects are represented by a collection of NURBS or T-Spline surfaces. But, to perform engineering analysis on real world problems, we must find a way to parameterize the volumes of these objects as well. This has proven to be difficult using traditional IGA, as the structured nature of trivariate NURBS and T-Splines limit their ability to create analysis suitable parameterizations of arbitrarily complex volumes. The TriGA (Triangular IGA) project aims to overcome this challenge by generalizing Isogeometric Analysis to triangles and tetrahedra. Currently, TriGA is capable of automatically creating high-quality, higher-order triangular meshes that exactly match arbitrary 2D geometries defined by NURBS curves. Moreover, TriGA enables semi-automatic mesh generation in three dimensions for most classes of geometries, and a clear plan exists for developing automatic robust meshing capabilities in the near future. These higher order meshes are made up of rational Bernstein-Bezier triangles in 2-D and tetrahedra in 3-D. The finite element subroutines for these patches are flexible and general purpose, and can support a variety of finite element methods, such as Galerkin and Discontinuous Galerkin methods. We demonstrate that these meshes are analysis suitable by solving the steady heat equation and linear elasticity equation over a variety of geometries using Galerkin’s method, as well as wave propagation using the Discontinuous Galerkin method.

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Title: Mechanical Property Characterization of Rate and Temperature-Dependent Short Fiber-Filled Polymer Composites

Author(s): Jaesung Eom, Don Robbins, Ravi Burla, *Autodesk*.

To predict the mechanical performance of fiber filled plastics, accurately accounting for the effect of fiber orientation is essential. This requires two conditions: 1) correct representation of the anisotropic material response in the local fiber direction, and 2) accounting for the spatial variation of the local fiber direction throughout the model. The first can be fulfilled by multiscale material modeling by homogenizing the response of microstructure. The second condition can be satisfied by mapping local fiber orientation distribution from injection molding simulation. Most applications of injection molded thermoplastic composites require good performance over a range of temperatures and deformation rates; therefore, simulations must account for the effects of temperature as well as strain rate. In this study we develop a simple interpolation and robust optimization techniques to represent and to characterize the nonlinear material properties of rate and temperature dependent short fiber composite for nonlinear finite element modeling. The application of multiscale modeling consists of a homogenization step and a decomposition step. An incremental Mori-Tanaka micromechanical model is formulated from matrix and fiber properties for an aligned microstructure geometry. The homogenized composite properties are subsequently modified by the fiber orientation tensor to account for the actual local distribution and orientation of the fibers. Then the homogenized composite strain increments from structural finite element code provide the average strain increments in the plastic matrix constituent material through the decomposition step. The present multiscale material model has at least 9 parameters to be determined. More precisely, there are four elastic constants for the matrix and fiber constituents, four plasticity constants for the matrix constituent and one constant for the effective strength of the matrix constituent. To represent effects of temperature and strain rate, we construct a simple 1st order interpolation function of temperature and loading rate for these 9 parameters; however, this method places high demands on the quality of the model coefficient fitting process. To fit the parameters, we use adaptive simulated annealing which statically finds the best global fit of a nonlinear, constrained, nonconvex cost-function. This algorithm permits an annealing schedule for “temperature” T decreasing exponentially in annealing-time k, $T = T0 \exp(-ck1/D)$. The introduction of re-annealing also permits adaptation to changing sensitivities in the multi-dimensional parameter-space. We tested this new scheme on the tensile behavior of extruded short E-glass fiber reinforced polyamide-6 composite sheets under different temperature 21.5°C, 50°C, 75°C, 100°C and different strain rates (0.05/min, 0.5/min, 5/min).

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Title: The Mechanics of Airway Obstruction and Characterization of Folding in Chronic Lung Disease

Author(s): Mona Eskandari, Ellen Kuhl, *Stanford U.*.

More than a quarter of the adult population is affected by chronic lung disease. Mechanically, the occlusion of the airways is a classical instability problem attributed to pressure and growth: airway constriction due to the thickening and contraction of the smooth muscle surrounding the airway wall acts as an induced pressure, and airway inflammation due to the influx of cells at the inner airway wall lining acts as an induced growth [1]. These mechanisms trigger mechanical instability of the airway wall, initiating inward folding and progressive airflow obstruction. Since the number of folds has been correlated with the degree of occlusion, pressure and growth buckling modes in the airways have been extensively studied for the limiting case of idealized, uniform, circular cross-sections [2, 3]. However, the behavior of imperfect, continuously branching airways, as found in the human body, remains unknown. Here we demonstrate the ability to predict instabilities and folding in three-dimensional patient-specific airways using the nonlinear field theories of mechanics. We perform systematic parametric studies, introduce a surrogate measure for lumen narrowing for non-symmetric geometries, and verify the relationship between lumen narrowing and folding patterns to quantify the risk of airway obstruction. Using finite element analysis for a growing bi-material structure with a stiff inner mucosal layer and a soft outer submucosal layer, we simulate pressure and growth loading on select three-dimensional Y-branch segments generated from magnetic resonance images of airway contours. Our results suggest that folding and obstruction due to pressure and growth are insensitive to the specific airway geometry; essentially, the mucosal thickness, submucosal thickness, and mucosal to submucosal stiffness ratio dictate the degree of airflow obstruction. We find that the impact of these parameters on the folding pattern is sensitive to the loading mechanism. Furthermore, we demonstrate that the inherent imperfections of patient-specific geometries cause fewer folds and greater airway occlusion when compared to idealized geometries. Our results agree with clinical observations and could help explain the mechanics of airway obstruction in chronic lung disease. [1] M. Eskandari, M.R. Pfaller, and E. Kuhl. On the role of mechanics in chronic lung disease. Materials 6:5639-5658, 2013. [2] R. K. Lambert. Role of bronchial basement membrane in airway collapse. J. Appl. Physiol. 71:666-673, 1991. [3] B.R. Wiggs, C.A. Hrousis, J.M. Drazen, and R.D. Kamm. On the mechanism of mucosal folding in normal and asthmatic airways. J. Appl. Physiol. 83:1814-1821, 1997.

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Title: Amplitude-Preserving Propagators to Improve the Efficiency of Full Waveform Inversion

Author(s): Mehran Eslaminia, *Bentley Sys.*; Murthy Guddati, *North Carolina State U.*.

Full waveform inversion (FWI) is aimed at predicting the substructure by minimizing the misfit between recorded data at the surface and simulated reflections. FWI is typically based on gradient-based optimization and involves three main steps. First, the misfit function is computed by solving full wave equation for all sources. Second, the gradient vector is estimated by cross-correlating the forward-propagated source wavefield and back-propagated (adjoint) wavefield. The third step involves inverting Hessian matrix to determine the descent direction. For large-scale problems, the descent direction is inexactly determined using a matrix-free conjugate gradient method which requires computing Hessian-vector products. FWI based on such an inexact Newton method requires numerous wave simulations at each iteration: one for computing the residual, one for estimating gradient and two for each Hessian-vector multiplication. Given the high-frequency nature of the problem, the forward simulations involve large number of unknowns, necessitating the use of iterative methods such as Krylov subspace methods. Unfortunately, these methods typically show very slow convergence for wave propagation problem due to the oscillating nature of the solution. In this study, we propose a novel approach, named amplitude-preserving propagators, to approximately solve wave propagation in the frequency domain [1]. The method involves partitioning the domain into horizontal slabs and solving each slab sequentially, which is facilitated by special interface conditions. It is shown that the proposed method results in accurate amplitudes for forward propagation and primary reflections and is hence called the amplitude-preserving propagators. This novel solver significantly increases efficiency of FWI in three different ways. Amplitude-preserving propagator is first implemented as a preconditioner to iteratively solve full-wave equation to accurately compute the residual. We observe that efficiency of the proposed preconditioner is not affected by frequency, discretization size and number of partitions. Second, the proposed method is used to estimate the gradient vector by approximately solving adjoint wavefield. Third, this method is used to approximately estimate Hessian-vector multiplication in FWI framework. We show that the convergence rate of FWI remains unchanged when the proposed approximation is used, thus leading to significant increase in efficiency. The performance of amplitude-preserving propagators is illustrated using a variety of acoustic and elastic wave propagation problems. References: [1] M. Eslaminia (2014), Amplitude-Preserving Propagator and Its Applications in Computational Wave Propagation and Seismic Imaging, Doctoral Dissertation, North Carolina State University.

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Title: Coherent Interface Elasticity Theory Accounting for Damage

Author(s): Ali Esmaeili, Paul Steinmann, *U. Erlangen*; Ali Javili, *Stanford U.* .

Interfaces can play a dominant role in the overall response of a body. The importance of interfaces is particularly appreciated at small scales due to the large interface area to volume ratio. From the mechanical point of view, this scale dependent characteristic can be captured by endowing the interface with its own elastic resistance as proposed by the interface elasticity theory. This theory proves to be an extremely powerful tool to explain the size-effect and to predict the behavior of nano-materials. To date The interface elasticity theory only accounts for the elastic response of the interface and obviously lacks an explanation for inelastic interface behavior such as damage or plasticity. The objective of this contribution[3] is to modify the interface elasticity theory to account for the damage of coherent interfaces. It follows the work of Javili and Steinmann [1, 2] by providing an extension to the continuum mechanics formulation which accounts for interface structures to include the effects of material degradation both on the interface and in the bulk using continuum damage mechanics. A thermodynamically consistent interface elasticity theory with damage is proposed. A local damage model for the interface is presented and is extended to a non-local damage model. The non-linear governing equations and the weak forms thereof are derived. The numerical implementation is carried out using the finite element method and consistent tangents are listed. The computational algorithms are given in detail. Finally, a series of numerical examples are studied to provide further insight into the problem and key features of the proposed theory are carefully elucidated. [1] Javili, A., Steinmann, P., 2009. A finite element framework for continua with boundary energies. Part I: The two-dimensional case. Computer Methods in Applied Mechanics and Engineering 198 (27 - 29), 2198 – 2208. [2] Javili, A., Steinmann, P., 2010. A finite element framework for continua with boundary energies. Part II: The three-dimensional case. Computer Methods in Applied Mechanics and Engineering 199 (9 - 12), 755 – 765. [3] Esmaeili, A.,Javili, A., Steinmann, P., 2015. Interface elasticity theory accounting for damage. Part I: Coherent interfaces. Submitted.

13th U.S. National Congress on Computational Mechanics
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Title: Direct Evaluation of Unified Extended Splines

Author(s): Emily Evans, Ian Henriksen, *Brigham Young U.*.

We present methods for the direct evaluation of unified extended splines (UE-splines) for use in isogeometric analysis. Algorithms for knot insertion, degree elevation and Bézier extraction will be given and the numerical stability of the algorithms presented will be considered. We also present sample problems which illustrate the utility of using these splines in isogeometric analysis.

13th U.S. National Congress on Computational Mechanics
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Title: Isogeometric Structure-Preserving Methods for Magnetohydrodynamics and Fluid-Structure Interaction

Author(s): John Evans, Craig Michoski, *U. Colorado-Boulder*.

In recent years, structure-preserving methods have emerged as an attractive class of discretization methods for the numerical solution of partial differential equations (PDEs). By construction, structure-preserving methods preserve important mathematical and physical structure exhibited by a system of PDEs, such as topological constraints, conservation or balance laws, symmetries, and maximum principles, for every level of discretization and every set of system parameters. As these methods automatically preserve the basic laws of physics, they far outperform classical methods in terms of accuracy and robustness, especially for coarse meshes. These methods have been applied with much success across a broad range of single-physics systems, including Hamiltonian mechanics, electromagnetics, and laminar incompressible and compressible fluid flow. In this talk, we will present a class of novel isogeometric structure-preserving methods for the computational analysis of complex fluid flow. The focus of the talk will be magnetohydrodynamics and fluid-structure interaction, but the overarching aim is to develop a unifying framework for the construction and analysis of structure-preserving methods for multi-scale and multi-physics systems. The proposed framework is built upon the emerging field of isogeometric discrete differential forms, a novel approach to the discretization of PDEs which constitutes a natural framework for the approximation of vector fields, such as the velocity or magnetic field. When these forms are applied to the solution of the incompressible Navier-Stokes equations, it has been shown the resulting scheme exhibits pointwise mass conservation and local conservation of momentum, energy, and enstrophy. When applied to the solution of the incompressible magnetohydrodynamics equations, the resulting scheme yields divergence-free velocity and magnetic fields. Such a scheme automatically conserves total energy and cross helicity, two quantities of critical importance in magnetohydrodynamic turbulence. Moreover, when isogeometric discrete differential forms are applied to the solution of fluid-structure interaction problems, the resulting scheme exhibits pointwise mass conservation on the time-evolving fluid domain, even in the presence of large displacements. We will give a brief overview on how to construct isogeometric structure-preserving methods for complex fluid flow, discuss their mathematical properties in the context of magnetohydrodynamics and fluid-structure interaction, and present basic numerical results illustrating the promise of this new technology.

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Title: Discontinuous Petrov-Galerkin Approach to Topology Optimization in Fluid Mechanics

Author(s): Anton Evgrafov, *Norwegian U. Sci. & Tech.*.

The need for efficient algorithms for solving large scale topology optimization problems is well recognized, in particular owing to advances in additive manufacturing technologies, which have made it possible to utilize topology optimization not only at the conceptual and preliminary but also at final design stages. Nevertheless, the construction of efficient algorithms for these problems is complicated by the nature of topology optimization. Indeed, the huge number of design and state variables, the presence of PDE constraints, and the non-convexity of these optimization problems all contribute to the fact that a universal robust and efficient algorithm for solving these problems is yet to be found. Our starting point in this work is a recent algorithm based on formulating the topology optimization problem in the state space, which has proved to be very efficient for self-adjoint problems in fluid mechanics [1]. We extend this algorithm by utilizing a least-squares type discretization, namely the discontinuous Petrov-Galerkin method with optimal test functions [2], on the first order optimality conditions. This provides us with a natural merit function even for non-selfadjoint problems, which is efficienly locally computable owing to the utilization of broken test spaces in this discretization strategy. Furthermore, this puts the overintegration strategy utilized in [1] to another good use in the element-wise inversion of the Riesz map associated with the test space, and simplifies the adaptive refinement in the context of topology optimization. In the presentation we will explain the method and present its performance on some benchmarking problems in topology optimization of fluid flows. References: [1] A. Evgrafov, On Chebyshev’s method for topology optimization problems of Stokes flows, Structural and Multidisciplinary Optimization, Online First (DOI: 10.1007/s00158-014-1176-x), 2015. [2] L. Demkowicz, J. Gopalakrishnan, A class of discontinuous Petrov–Galerkin methods. Part II: optimal test functions Numer. Methods Partial Differential Equations, 27, pp. 70–105, 2011.

13th U.S. National Congress on Computational Mechanics
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Title: Estimation of Error for Coarse-Grained Models of Atomic Systems

Author(s): Danial Faghihi, Kathryn Farrell, J. Tinsley Oden, *UT Austin*.

The most common method of constructing reduced-order models in all of computational science involves the use of coarse-grained models of atomic systems, whereby systems of atoms are aggregated into "beads" to reduce the number of degrees of freedom and to lengthen the time scales in which the evolution of events are simulated. The issue of central importance in developing coarse-grained models is the accuracy with which they approximate key features of the atomistic system. This talk will present a general framework for adaptive validation of coarse-grained models of atomistic systems. An algorithm referenced to as the Occam-Plausibility algorithm, is presented for systematically arriving at a valid model among a class of coarse-grained models. In addition, a posteriori estimates of modeling error is derived in constructing coarse-grained models of atomistic systems. Computable error estimates for the coarse-graining method are developed with respect to specific quantities of interest. The theoretical results are illustrated on simple model problems of polyethylene chain under prescribed deformation, in which the quantity of interest is the locally averaged displacement of atoms. The results of numerical experiments are presented to con firm the effectiveness of these adaptive methodology.

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Title: A Hybrid Peridynamics-SPH Simulation of Soil Fragmentation by Blast Loads of Buried Explosive

Author(s): Houfu Fan, Shaofan Li, *UC Berkeley*.

In this work, we employ both the state-based peridynamics and the smoothed particle hydrodynamics (SPH) to simulate soil fragmentation/ejection induced by the blast of buried explosives. We use peridynamics representation to model soil medium, and we use SPH representation to model explosive gas. The key of the simulation is the coupling of the two. In the peridynamics-SPH computational domain, there is an interphase zone, in which a peridynamic particle can have SPH particles within its own horizon, while an SPH particle can have peridynamic particles within its supporting domain. The interactions of the peridynamic and SPH particles in this interphase zone are discussed. By assuming the equivalence of the two methods in the current configuration, we study how to choose simulation parameters that can seamlessly couple the two methods. A Drucker-Prager plasticity soil model at finite strain is used for soil medium and a charge model of equation of state is used to model the TNT explosive. Numerical examples are carried out to simulate soil fragmentation/ejection induced by the shock waves from the blastic loadings of the buried explosive.

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Title: Large Eddy Simulation for Entrainment and Suspension of Fine Sediment in Open Channels

Author(s): Hongwei Fang, Yan Liu, *Tsinghua U.*.

This paper investigates how sidewalls affect the entrainment, suspension and transport of fine sediments by means of large eddy simulations. A new sediment entrainment boundary is formulated and adopted. This boundary condition is validated by two physical experiments of fine sediment erosion and a fairly good agreement between measured data and computed results are got. Then three open channel flow cases with different aspect ratios (A=B/H=2,4 and infinite, respectively) are performed to study the influence of sidewalls on sediment erosion. Results show that the channel aspect ratio is the determining factor for the development, strength and distribution of turbulence-driven secondary flow. And the secondary flow greatly influences the cross-section distribution of primary flow, coherent structures and vertical flow, which results in a non-uniform erosion of fine sediment particles over the cross-section. In the streamwise direction, cross-averaged sediment concentration increases faster in the channel with A=2 than the ones with A=4 and infinite, which means a strong sediment erosion in the narrow channel. Sediment entrainment is found to be closely related to the vertical velocity, which can be clearly recognized by plotting the velocity vector on instantaneous sediment concentration. Moreover, vortices are visualized to show details of sediment pick-up by these structures. A spiral sediment concentration distribution is observed on the vortices, i.e. concentration is higher at the upward flow side of vortex and lower at the downward flow side, which reveals the importance of vortices on transporting sediment into the outer flow field.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Bayesian Framework for Adaptive Selection, Calibration, and Validation of Coarse-Grained Models of Atomistic Systems

Author(s): Kathryn Farrell, J. Tinsley Oden, Danial Faghihi, *UT Austin*.

Important advances in material science, biology, nanomanufacturing, drug design, and in many other fields, brought about by developments in computational modeling and simulation, high-performance computing, and experimental science, have dramatically expanded interest in the use of atomistic models to study a wide variety of physical phenomena and to analyze the behavior of many engineering and medical systems. Although the universally accepted approach for modeling atomistic systems is to employ molecular mechanics simulations in the form of either molecular dynamics or Monte Carlo sampling, implemented using any of several well-documented and well-tested codes, the enormous size and complexity of systems of interest far exceed the capabilities of today's largest super computers or even those envisioned decades into the future. Coarse-grained (CG) models of atomistic systems, in which groups of atoms are aggregated into larger units to reduce the number of degrees of freedom, have been used for decades in significant technological and scientific applications. The development of a rigorous mathematical, physical, and statistical foundation for the process of coarse graining, including calibration, validation, and assessment of predictability of CG models, is, hence, a goal of great importance in computational science. In this study, Bayesian methods for statistical calibration, validation, and model selection are used to develop basic principles for constructing CG models. A general adaptive modelling algorithm, the Occam-Plausiblity (OP) Algorithm is described, for the selection and validation of predictive CG models. The method incorporates methods of sensitivity analysis, information theory, the Bayesian notion of model plausibility, and the principle of Occam's Razor. Applications to polymeric materials are presented

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Title: Optimizing an Elastic Wave Propagation by Means of a Roofline-Based Strategy on Xeon Processors

Author(s): Mauricio Hanzich, Albert Farres, *Barcelona Supercomputing Center* ; Felix Rubio, *Techn'l. U. Catalonia*.

Full wave elastic propagation is expensive both, computational- and development-wise. Hence, maximizing the efficiency of your propagation code at the minimum development cost is important. For that, a mechanism to evaluate the current efficiency of your application and the maximum attainable is needed. Within this work we will show our experience in enhancing an elastic wave propagation on Xeon® processors by means of a roofline-directed optimization strategy [1]. This will provides the means to evaluate which kind of optimizations to apply and when to stop the optimization process. The roofline model [2] provides an insight of your application behavior by placing its performance into a graphical representation bounded by both the maximum (attainable) flops and the memory bandwidth. In order to use the model you need to measure your application operational intensity and the efficiency, in GFlops. As the model impose a limit on the upper performance you can get regarding the operational intensity obtained for your application, it eases the selection of the optimizations to be applied and their order. This in turn let the developer reduce the optimization development cost at the time that produces the better performance enhancement that can be achieved for the application. In this work we apply the roofline model to an elastic wave propagation application for both, the propagation kernel and the whole application including the absorbing boundary conditions (ABCs), source insertion, output interpolation, etc. We have started the optimization process by enhancing the ABCs by merging the stencil and absorption process, then the NUMA architecture of our Xeon® environment was considered to enhance performance, after that some prefetching was introduced to increase bandwidth usage and finally a blocking scheme was included to increment the operational intensity of the stencil kernel. Our results show that by applying the roofline model we were able to halve the execution time of the whole application within a restricted margin of time. This in turn, demonstrates the usefulness of such kind of models to guide the optimization process of an HPC application by letting select and prioritize the proper strategies for performance enhancing. [1] Mauricio Hanzich. “Roofline-Based Optimization of Elastic Wave Propagation”. SHPCP Theater at SEG Annual Convention, Denver, Co, USA. October 2014. [2] Williams Samuel, Andrew Waterman, and David Patterson. "Roofline: an insightful visual performance model for multicore architectures." Communications of the ACM 52.4 (2009): 65-76.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Performance of Finite-Element Models of Turbulent Air/Water Flow in Coastal and Hydraulic Applications

Author(s): Christopher Kees, Matthew Farthing, Aron Ahmadia, *USACE* ; Jed Brown, Barry Smith, *Argonne Nat'l. Lab.*; Aggelos Dimakopolous, Eleni Zve, Giovanni Cuomo, *HR Wallingford Ltd*.

Capturing turbulent air/water flows around structures is critical for many coastal and hydraulic applications. The concept of fully three-dimensional modeling of these flows for real-world engineering analysis is gaining acceptance among the community and practitioners. However, the computing resources required for simulating large-scale systems while resolving relevant physical processes remains a major barrier to widespread adoption of the overall approach. Here, we consider level-set based methods for modeling two-phase Navier-Stokes systems using stabilized finite element approximations. We evaluate their performance for a series of problems involving free-surface flows around coastal structures. We focus in particular on recently developed preconditioners that use Schur-complement factorizations to exploit the block structure of the operators arising from the two-phase Navier-Stokes system.

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Title: Dynamic Assessment of Stress Field Behavior Induced by Fracture Tip Propagation in Quasi-Brittle/Ductile Shale Reservoirs: A New Approach Based on Modified Theory of Critical Distances

Author(s): Ebrahim Fathi, Andrew Jenkins, Liliia Reddy, *West Virginia U.*.

Hydraulic fracturing is a complicated coupled process, where fracture propagation in a solid medium driven by pressurized fluid, is used for reservoir stimulation. This process changes the initial state of stress in the field creating more contact area but can also lead to discontinuity failure/ fault reactivation. Advanced knowledge on dynamics of magnitude and direction of change in in-situ field stress is essential for optimization of multiple hydraulic fracturing design and minimization of the environmental impact and footprint associated with these activities. An interesting topic in the aspect of fracture assessment is the use of the Theory of Critical Distances (TCD) for assessment of stress concentration features in the vicinity of notched materials. These features of the components allow for a stress concentration to be developed much in the same way that occurs around a discontinuity or material flaw. The Theory of Critical Distances (TCD) envelopes the idea of a critical region close to the crack tip and can be modified and used to predict the dynamics of failure of stress containing bodies under static or dynamic loading “Mode I” loading. In this study, in-house fully coupled hydraulic fracturing simulator “HFWVU” based on finite element method and LEFM is used to model hydro-mechanical interactions of single and multiple hydraulic fractures generated simultaneously or sequentially. The modified TCD is then used for quasi-brittle and ductile shale reservoirs to assess stress field behavior around the fracture tip, in that there is a critical distance in which interaction occurs between the fracture tip and the surrounding stress fields. Application of modified TCD with maximum Von Mises stress clearly defines the dynamics of failure envelope around the fracture tip. This behavior can be idealized such that the maximum Von Mises stress emanates from the fracture tip creating a critical angle with fracture plane or fracture tip. This critical angle can be used to justify the stability of the reservoir or in regard to stress reorientations that are seen around propagating fractures. These reorientations can affect the geometry and relative stress distributions surrounding adjacent fracture propagation by either easing or impeding the ability of the fracture to propagate. In this paper we developed a robust and highly accurate model to assess the dynamic stress field around single and multiple-hydraulic fractures generated simultaneously or sequentially that releases the need for costly and time consuming experiments to characterize stress vs strain dynamic behavior of qusi-Brittle/Ductile Shale samples.

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Title: Large-Scale Inversion of the Lamé Parameters in PML-Truncated Domains Using Full-Waveforms

Author(s): Arash Fathi, Loukas Kallivokas, *UT Austin*.

We are concerned with high-fidelity subsurface imaging, which commonly arises in geotechnical site characterization and geophysical explorations. Specifically, we attempt to image the spatial distribution of the Lamé parameters in semi-infinite, three-dimensional, arbitrarily heterogeneous formations, using surficial measurements of the medium's response to probing elastic waves originating from the free surface. We use the complete waveform response of the medium to derive the inverse medium problem, by using a partial-differential-equation (PDE)-constrained optimization approach, directly in the time domain. In order to resolve the forward problem, we use a recently developed hybrid finite element approach, endowed with perfectly-matched-layers (PMLs) to arrive at a finite computational domain. Specifically, a displacement-stress formulation for the PML is coupled with a standard displacement-only formulation for the interior domain, resulting in a computationally optimal procedure. Time-integration is accomplished by using an explicit Runge-Kutta method, which is well suited for large-scale problems on parallel computers. We report numerical experiments for prototype heterogeneous formations, using both noiseless and highly-noisy synthetic records. We also report on the characterization of the NEES site in Garner Valley, CA, using field records and compare the resulting imaging based on the full-waveform method against the profiling obtained by the SASW method. The new developments in the three-dimensional forward and adjoint solvers, their implementation on parallel architectures, and their integration to current field technologies, constitute the primary contributions of this work. Keywords: Full-waveform inversion, PDE-constrained optimization, Perfectly-matched-layer (PML), Explicit time-stepping, Mixed-field finite elements, Field data

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Title: Vibration Analysis of Carbon Nanotube-Reinforced Doubly-Curved Shell Panels

Author(s): S. Ahmad Fazelzadeh, Saleh Pouresmaeeli, *Shiraz U.*.

Carbon nanotube (CNT) is a well-known nanostructure with extraordinary mechanical, electronic, transport, and thermal properties. Due to the incomparable mechanical properties of carbon nanotubes, these nanostructures become ideal candidate for reinforcing of polymer composites. It is shown that adding CNT even at very low volume fractions, improve mechanical properties of carbon nanotube reinforced composites (CNTRCs) significantly. The CNTs in the CNTRCs can be distributed uniform or functionally graded. In functionally graded case, properties of the composite change smoothly from one surface to the other. This kind of composite is known as functionally graded carbon nanotube-reinforced composite (FG-CNTRC). Based on their special properties such as high stiffness and light weight, they become subjects of primary interest in recent studies. In spite of the researches in the area of the vibration of the FG-CNTRC, vibration analysis of uniform and functionally graded CNTRC doubly-curved moderately thick shell panels is not investigated so far. In this paper, the material properties are estimated based on rule of mixture and equations of motions are derived via first order shear deformation theory. Hence, five complex and coupled equations with respect to displacements are derived. Due to complexity and coupling of the governing differential equations, it is challenging to attain the closed-form solution and Galerkin's method is applied to solve coupled equations of motions simultaneously. To validate the accuracy of the results, comparison are done with results found in the literature. To show vibrational characteristics of FG-CNTRC, frequency changes with respect to volume fraction, thickness ratio and side-to-radius ratio for various doubly-curved shell panels such as cylindrical, spherical and general doubly-curved panels are investigated. It is shown that frequencies are increased with the increase of volume fractions and thickness-to-side ratio. Moreover, by increasing side-to-radius ratio, frequencies of various FG-CNTRC are increased on the other hand differences among frequencies of different kinds of FG-CNTRC are decreased.

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Title: A Comparison of Standard and Iso-Geometric Element for Structural Vibrations

Author(s): Carlos Felippa, *U. Colorado*.

A Comparison of Standard and IsoGeometric Elements for Structural Vibrations Carlos A. Felippa Professor, Aerospace Engineering Sciences and Center for Aerospace Structures, University of Colorado, Boulder, CO, USA, email: carlos.felippa@colorado.edu There has been relatively few studies comparing the performance of standard andisogeometric (iso-G) finite elements in structural dynamics. An obvious reason is the relative newness of the latter; another is the restriction to limited classes of standard models. The aim of this paper is to provide comparisonsin the linear elastic, one-dimensional case, in which finite elements model a prismatic bar member. This restriction is due to practical reasons: (1) Analytical solutions for the continuum case are readily available; (2) Mass matrix templates have been thoroughly developed only in the 1D case; (3) Thorough symbolic analysis can be performed using Mathematica; (4) Multidimensional complications such as mesh directionality and the intrusional effect of material parameters is avoided. A FEM discretization is labeled iso-G if it is based on the isogeometric approach, in which NURB splines extend over adjacent element regions. Iso-G elements overlap on assembly. Elements with strict local support are labeled standard, in accordance with historical order of appearance. Standard elements are developed here with the template approach. Templates are algebraic forms for the mass and stiffness matrix. Forms are parametrized with the aim of including a range of standard admissible elements of a given type. By given type is meant that the template is applicable to elements of specific geometries with identical nodal and DOF configuration. By admissible is meant that the model is convergent and stable. If the element type is sufficiently simple, the range may include all admissible ones, in which case it is called a general template. The set of parameters is the template signature. Choosing numerical values for the signature produces template instances. Well known element instances are obtained for specific signatures, but so do an infinity of other ones. It is not presently known whether templates can be constructed for iso-G elements.The fact that the NURBS choice of shape functions depend on nonlocal features such as the position of the element within the mesh as well as interknot continuity complicates parametrization. This paper focuses on standard FEM models of prismatic bar elements with 2 and 3 nodes.The comparison includes vibration spectra as wellas dispersion diagrams. Given a vibration benchmark with known solutions,the vibration frequency spectral ratio diagram (VFSRD) list-plots the ratio of all natural frequenciesgiven by the discrete FEM model to the corresponding continuum values. The vibration frequency spectral accuracy (VFSAd list-plots the number of correct digits in the computed frequencies. A related diagram, called VMSAD for Vibration Mode SpectralAccuracy Diagram, quantifies eigenvector accuracy.Whereas VFSRD, VFSAD and VMSAD focus attention on vibration performance, dimensionless dispersion diagrams (DDD) that relatefrequency to wavenumber picture expected behaviorin wave propagation analysis. Standard elements are formulated interms of mass and stiffness templates. Iso-G elements are constructedwith NURBS spline shape functions. The main difference as regards model assemblyis that standard elements do not overlap whereas iso-G elements do. Linear and quadratic elements of both types are investigated. It is found that the use of templates allows customization to specific behavior, and that customized templates can be made to display performance similar to that of the iso-G elements with identical number of degrees of freedom.

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Title: Damage-Dependent Bio-Heat Transfer Modeling in Thermal Therapy with Consideration of Perfusion Field

Author(s): Cliff J. Zhou, Robert Moser, *UT Austin*; Yusheng Feng, *UTSA*.

In thermal therapeutic treatment planning and optimization, it is essential to characterize tissue properties in order to model bio-heat transfer in both healthy and cancerous tissues. However, it is challenging to determine thermal conductivity and perfusion parameter when these properties are evolving due to thermal damage of tissues during the thermal treatment. In this talk, we present a damage-dependent perfusion model, where capillary perfusion field changes as thermal damage accumulates, based on a general model derived from the fundamental principles of continuum mixture theory. Specifically, the permeability and heat transfer coefficient of tissue are considered to be dependent on the state of tissue damage. We also consider the inter- and intra-patient variations of the tissue porosity and blood flow rate due to different physiological states and pathological conditions. The results show that the temperature fields are quite different between damage-dependent bio-heat transfer model and traditional Pennes Bio-heat transfer models, when tissue properties vary due to thermal damage as in the real surgical situations. Moreover, we will present critical range of model parameters so that the damage-dependency has large effect on perfusion, which in turn will affect the reliability of treatment planning based on traditional modeling methodology.

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Title: Characterization of True Stress-Strain Behavior of Plastic Materials via Inverse Finite Element Analysis

Author(s): Jie Feng, Yijian Lin, Jeff Zawisza, Todd Hogan, Rashi Tiwari, Sam Crabtree, Brandon Weinlander, *Dow Chem'l. Co.*.

Characterization of the true tensile behavior of plastic materials such as high density polyethylene (HDPE) is difficult, not only due to their tendency to develop uncontrolled necking, but also due to their premature fracture that often occurs during the process of necking propagation. In this study, the tensile test was conducted on the modified tensile bars with 1% width reduction in the middle, which ensured that the necking always initiated at the target location. The true stress-strain behavior of the HDPE resins was obtained via Inverse Finite Element Analysis (FEA) along with the local strain measurement. Effect of each section of the true stress-strain response on the measured engineering stress-strain curve was also investigated. Furthermore, this study explored the feasibility of using inverse FEA to characterize the true tensile behavior of the injection molded parts with an irregular geometry. Due to the irregularity of the sample geometry, multiple strain stress responses could be used to fit one single experimental result. Hysteresis tensile test was employed to exclude unreasonable results and obtain the unique true stress-strain response of the material. It was noticed that the strain hardening behavior of the molded plastic parts varied with the processing conditions. Through this study, it is also demonstrated that the measurement accuracy of polymer material characterization can be significantly improved by utilizing numerical simulation in an inverse manner.

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Title: Optimal Experimental Design in the Presence of Nuisance Parameters and Model Error

Author(s): Chi Feng, Youssef Marzouk, *MIT*.

The optimal selection of experimental conditions is essential to maximizing the value of data for inference and prediction. We propose an information theoretic framework and algorithms for robust optimal experimental design with simulation-based models, with the goal of maximizing information gain in targeted subsets of model parameters, e.g., parameters of interest, particularly in situations where experiments are costly. By ignoring the information gain in nuisance parameters, our framework can explore the tradeoff in information gain between subsets of model parameters present in many experimental design problems. Our framework employs a Bayesian statistical setting, which naturally incorporates heterogeneous sources of information. An objective function reflects expected information gain from proposed experimental designs. Adaptive importance sampling techniques are used to evaluate the expected information gain, and stochastic approximation algorithms make optimization feasible for computationally intensive and high-dimensional problems. A key aspect of our framework is the inclusion of model discrepancy terms used to capture model error, which we treat as nuisance parameters. We illustrate the approach via several model problems and misspecification scenarios. In particular, we show how optimal designs are modified by allowing for model error, and we evaluate the performance of various designs by simulating data from more "realistic," or higher-fidelity models not considered explicitly in the optimization objective.

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Title: Strain-Induced Phase Transformation Under Compression and Compression and Torsion in a Diamond Anvil Cell: Simulations of a Sample and Gasket

Author(s): Biao Feng, *Iowa State U.*.

Combined high pressure phase transformations (PTs) and plastic flow in a sample within a gasket compressed in diamond anvil cell (DAC) or compressed and twisted in rotational DAC are studied using finite element method (FEM). The key point is that phase transformations are modelled as strain-induced, which involves a completely different kinetic description than for traditional pressure-induced PTs. Corresponding microscale constitutive model is presented. Contact sliding with Coulomb and plastic friction at the boundaries between the sample, gasket, and anvil is taken into account. A comprehensive computational study of the effects of the kinetic parameter, ratio of the yield strengths of high and low-pressure phases and the gasket, sample radius and initial thickness on the PTs and plastic flow is performed. A new sliding mechanism at the contact line between the sample, gasket, and anvil called extrusion-based pseudoslip is revealed, which plays an important part in producing high pressure. Strain-controlled kinetics explains why experimentally determined phase transformation pressure and kinetics (concentration of high pressure phase vs. pressure) differ for different geometries and properties of the gasket and the sample: they provide different plastic strain, which was not measured. Utilization of the gasket changes radial plastic flow toward the center of a sample, which leads to high quasi-homogeneous pressure for some geometries. For transformation to a stronger high pressure phase, plastic strain and concentration of a high-pressure phase are also quasi-homogeneous. This allowed us to suggest a method of determining strain-controlled kinetics from experimentation, which is not possible for weaker and equal-strength high-pressure phases and cases without a gasket. Effect of torsion is studied in detail. Some experimental phenomena are reproduced and interpreted. Developed methods and obtained results represent essential progress toward the understanding of PTs under compression and compression and torsion in the DAC. This will allow one optimal design of experiments and conditions for synthesis of new high pressure phases.

13th U.S. National Congress on Computational Mechanics
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Title: Assessing Structural Response to Intense Loading Environments

Author(s): Robert Ferencz, Anthony DeGroot, James Durrenberger, Jerry Lin, Michael Puso, Jessica Sanders, Robert Sherwood, Edward Zywicz, *LLNL*.

Structural response assessments at LLNL include high- and hyper-velocity impacts, fragmentation, infrastructure vulnerability and other highly transient events. The ParaDyn code leverages the core explicit transient dynamics capabilities of DYNA3D and extends them to productively use hundreds and thousands of processing units. We highlight a series of applications by our users and collaborators. Some leverage our emerging capability to co-execute two codes via an embedded mesh approach to cooperatively solve a complex problem. Snapshots of recent computational mechanics research by the code development team are offered to illustrate such capabilities and ongoing challenges. Observations will also be offered on some of the issues raised by the emerging wave of next-generation hardware architectures. References [1] A.J. De Groot, R.J. Sherwood, J.K. Durrenberger, “ParaDyn, a Parallel Nonlinear Explicit, Three-Dimensional Finite-Element Code for Solid and Structural Mechanics: Version 14.1”, Lawrence Livermore National Laboratory, LLNL-SM-660481, 2014. [2] M.A. Puso, J.D. Sanders, R.R. Settgast and B.T. Liu, “An embedded mesh method in a multiple material ALE”, CMAME, 245 pp. 273-289, 2012. [3] M.A. Puso, E.J. Kokko, R.R. Settgast, B.G. Simpkins and B.T. Liu “An embedded mesh method using piecewise constant multipliers with stabilization: mathematical and numerical aspects”, IJNME, submitted 2014. Acknowledgement This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Some work supported by the DoD HPC Modernization Program via participation in an HPC Software Application Institute at the Army Research Laboratory.

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Title: Multi-Scale Analysis of Stretched Plates by Coupling BEM and FEM and Considering Different Boundary Conditions for the RVE

Author(s): Gabriela Rezende Fernandes, *UFG* ; Jose Julio de Cerqueira Pituba, *UFG*; Eduardo Alberto de Souza Neto, *Swansea U.*.

A multi-scale modelling for analyzing the stretching problem of heterogeneous plates is presented. The macro-continuum, represented by the plate, is modelled by the BEM (Boundary Element Method) while the equilibrium problem at micro-scale (represented by the Representative Volume Element - RVE) is solved by a FEM (Finite Element Method) formulation that takes into account the Hill-Mandel Principle of Macro-Homogeneity. Each point of the macro-continuum is related to a RVE, whose equilibrium equation is written in terms of displacement fluctuation. The micro-to-macro transition can be made after solving the RVE equilibrium problem, by applying the volume averaging hypothesis of strain and stress tensors. Some numerical examples are then analyzed to show that the proposed formulation is a suitable tool for the analysis of stretched of plates composed of heterogeneous materials. To define the microstructure, different RVEs composed of an elasto-plastic matrix with inclusions or voids are considered. Three different boundary conditions for displacement fluctuation are imposed over the RVE: (i) linear displacements, (ii) periodic displacement fluctuation and (iii) uniform boundary tractions.

13th U.S. National Congress on Computational Mechanics
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Title: A Comparison of Hybrid and Standard Discontinuous Galerkin Methods for Output-Based Adaptive Simulations on Deformable Domains

Author(s): Krzysztof Fidkowski, *U. Michigan*.

High-order methods in CFD offer accuracy that is often superior to low-order methods, but at an increased computational expense. The hybridized discontinuous Galerkin (HDG) method offers savings in degrees of freedom and matrix size compared to the popular discontinuous Galerkin (DG) method, in particular at high orders of approximation. A fair way to compare these methods is in an output-based adaptive setting, in which mesh resolution is automatically prescribed from an estimate of the error in an output of interest. We consider such a comparison for unsteady CFD simulations, where adaptation in both space and time are required. In this talk, we first extend unsteady output-based adaptation techniques to high-order compressible Navier-Stokes simulations on deforming domains, discretized with HDG. We handle deforming domains through an arbitrary Lagrangian-Eulerian method, in which transformed partial differential equations are solved on a fixed reference domain to model the behavior on the deforming physical domain. We discuss details of HDG-specific aspects transformation, including stabilization and output calculation. The temporal discretization is DG in time, which lends itself to rigorous a posteriori error estimation using a fine-space discrete adjoint solution. Space-time error estimates drive metric-based static spatial and temporal refinement on unstructured spatial meshes and slab-based temporal nodalizations. We show accuracy and cost comparisons between adaptive DG and HDG simulations of two-dimensional flows governed by the compressible Navier-Stokes equations.

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Title: Dislocation Density Observations and Crystal Plasticity Modeling for Deformation of Alpha Iron

Author(s): David Field, Zhe Leng, *Washington State U.*; Nathalie Allain-Bonasso, Francis Wagner, *U. Lorraine*.

A polycrystalline alpha-iron sample was plastically deformed under uniaxial tensile stress at room temperature and a low strain rate. The microstructure of the deformed sample was analyzed using electron backscatter diffraction (EBSD). In addition, analysis employing a dislocation density based crystal plasticity finite element (CPFE) simulation was conducted using the initial measured sample texture. Both the experiment and the simulation results indicated localized plastic strain and dislocation patterning, which were controlled by the individual crystallite orientations and the grain boundary effects. The results also revealed that the level of concentrated stress at the grain boundaries depends on misorientation of the interface. Grain boundaries and triple junctions had higher hardening effects than the grain interiors.

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Title: Material Models and Responses at Micro- and Macro-Scales

Author(s): Mircea Grigoriu, *Cornell U.*; Richard Field Jr., John Emery, *Sandia Nat'l. Lab.*.

Material properties at micro-scale vary randomly in space and are best described by random fields. Under some assumptions on these fields, e.g., ergodicity and scale separation, material properties at this scale can be mapped into material properties at macro-scale. The latter properties, referred to as effective properties, are deterministic and are used in continuum mechanics. Material responses at micro- and macro-scales satisfy equations that have the same form but random and deterministic coefficients, i.e., stochastic and deterministic equations. Let $U(x)$ and $u_0(x)$, $x\in D$, be material responses at micro- and macro-scales, where D denotes the specimen domain. We assume that (1)~the source terms and boundary conditions of the equations for $U(x)$ and $u_0(x)$ coincide and are deterministic so that differences between these responses relate solely to material models and (2)~the probability law of the random fields characterizing micro-scale material properties is known and $U(x)$ constitutes the actual response. The continuum mechanics solution $u_0(x)$ is viewed as an approximation for $U(x)$. One of our main objectives is to assess the potential of the continuum mechanics solution as an approximation of the micro-scale solution. A natural requirement is that continuum solutions match micro-scale solutions on average, i.e., they are such that $u_0(x)=E[U(x)]$, $x\in D$, where $E[\cdot]$ denotes the expectation operator. Continuum solution with this property are said to be consistent. It is shown that continuum mechanics solutions may or may not be consistent depending on the problem and quantity of interest. Other metrics are considered to capture other aspects of the relationship between micro- and macro-scale solutions. Theoretical arguments, algorithms and numerical examples are presented to quantify similarities and differences between material responses corresponding to material models at micro- and macro-scales.

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Title: Dispersive Computational Continua

Author(s): Vasilina Filonova, Dimitrios Fafalis, Jacob Fish, *Columbia U.*.

The two primary objectives of the present work are: (i) to develop a variant of the computational continua formulation (C2)[1,2] with outstanding dispersive properties and (ii) to conduct its rigorous dispersion analysis. The ability of the C2 formulation to capture dispersive behavior stems from its underlying formulation that does not explicitly assume scale separation and accounts for microstructures of finite size. The dispersion study in heterogeneous elastic media with periodic microstructure has been conducted by both analytical and numerical approaches. The so-called analytical dispersion analysis is based on the Floquet-Bloch wave solution whereas the numerical dispersion analysis is based on the modal analysis of the discrete coupled fine-coarse-scale equations. The dispersive curves obtained from the dispersive C2 formulations were compared with the classical exact Floquet-Bloch wave solution, hereafter referred to as the reference dispersive curve. It has been observed that in the case the unit cell sizes being either half of the coarse-scale element size or equal to it, dispersive curves obtained by the dispersive C2 formulation are practically identical to the reference solution. For other cases, the dispersive C2 solution is in good agreement with the reference solution provided that the wavelength is resolved by at least two coarse-scale quadratic elements. The dispersion analysis results have been further verified by the wave propagation problem in a periodic heterogeneous medium with a wavelength comparable to the microstructural size. References: [1] J. Fish, V. Filonova, D. Fafalis, Computational continua revisited, Int. J. Numer. Meth. Engng. (2014), DOI: 10.1002/nme.4793. [2] J. Fish, S. Kuznetsov, Computational continua, Int. J. Numer. Meth. Engng., 84 (2010) 774-802.

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Title: The Future of LES and DNS in High-Performance Computing

Author(s): Paul Fischer, *U. Illinois*.

Petascale computing platforms currently feature million-way parallelism and it is anticipated that exascale computers with billion-way concurrency will be deployed in the early 2020s. In this talk, we explore the potential of computing at these scales with a focus on turbulent fluid flow and heat transfer in a variety of applications including nuclear energy, combustion, oceanography, vascular flows, and astrophysics. Following Kreiss and Oliger '72, we argue that high-order methods are essential for scalable simulation of transport phenomena. We demonstrate that these methods can be realized at costs equivalent to those of low-order methods having the same number of gridpoints. We further show that, with care, efficient multilevel solvers having bounded iteration counts will scale to billion-way concurrency. Using data from leading-edge platforms over the past 25 years, we analyze the scalability of state-of-the-art solvers to predict parallel performance on exascale architectures. With the end of frequency scaling, the principal avenue for increased performance is through greater concurrency, which favors solution of larger problems rather than faster solution of today's problems. We analyze these trends in order to shed light on the expected scope of next generation LES/DNS simulations and to provide insight to design requirements for future algorithms, codes, and architectures.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Deviatoric Shape of Concrete Failure Surface Based on Bezier Curves

Author(s): Paula Folino, *U. Buenos Aires*.

In this work the suitability of Bezier polynomials for representing an appropriate deviatoric shape to be considered mainly in failure surfaces and also in yielding surfaces of concrete like materials is explored. Three different options are evaluated, involving quadratic, cubic and rational quadratic Bezier curves, as an alternative to the classical and extensively used elliptical interpolation between the compressive and tensile meridians proposed by Willam & Warnke (1974). Like the latter, the three proposals lead to a deviatoric shape similar to a triangle with rounded corners, with a C1 continuity type. It is well known that failure and mechanical behaviour of concrete like materials depend on all the three invariants and therefore yielding and failure surfaces involving a circular deviatoric shape, neglecting the incidence of the third invariant, cannot accurately represent the main features observed in concrete experimental tests, particularly when low confinement levels and load scenarios leading to different Lode angles are considered. Several deviatoric shapes involving the third invariant have been proposed in the literature. Most of them present a lack of smoothness and therefore, are not convenient for numerical implementations. Among the proposals considering a C1 continuity type, outstands the above mentioned proposal by Willam & Warnke (1974), consisting in a deviatoric shape described by three ellipses. The motivation of this work aims to improve the available numerical tools for considering the third invariant in constitutive models for concrete. On the one hand, it has been demonstrated in Folino and Etse (2011) that when the elliptical interpolation fails to accurately predict peak stress under biaxial stress states particularly in the compression-compression quadrant, the numerical approach does not present any tool permitting to improve this accuracy, and thus, any contribution in this sense was the first objective of this work. On the other hand, the complexity involved in numerical approaches considering the third invariant usually discourages it application, and then, the second objective was to explore other possible mathematical descriptions of the deviatoric shape. Herein, three different types of Bezier curves are considered following these two main purposes. It is demonstrated that the rational quadratic type can be considered the most appropriate alternative to the elliptical interpolation. References [1] K. Willam and E. Warnke, “Constitutive model for the triaxial behavior of concrete”, Proc. Intl. Assoc. Bridge Struct. Engrg., Report 19, Section III, Zurich: 1-30 (1974). [2] P. Folino and G. Etse, “Validation of performance-dependent failure criterion for concretes”, ACI Materials Journal, Vol.108-3 (2011)..

13th U.S. National Congress on Computational Mechanics
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Title: Semi-Implicit Time Discretization of the Incompressible Navier-Stokes Equations: VMS-LES Modeling in a High-Performance Computing Setting

Author(s): Davide Forti, Luca Dedè, Simone Deparis, *EPFL*.

In this work, we consider the incompressible Navier–Stokes equations with Variational Multiscale–Large Eddy Simulation (VMS–LES) modeling of turbulence [1], with the focus being on their semi–implicit time discretization. We discretize the problem using the finite elements method in space and finite differences based on backward differentiation formulas (BDF) in time; the velocity and pressure variables at the coarse scales level, according to the VMS methodology [2], are represented by the same spaces of Lagrange polynomials. The nonlinear terms of the Navier–Stokes equations with VMS–LES stabilization are linearized by Newton-Gregory backward polynomials. In this way, at each time step, the full discrete problem only involves the solution of a linear system, which we numerically solve by the GMRES method with a suitable parallel multigrid preconditioner. We validate the proposed numerical scheme by solving reference problems at high Reynolds numbers, namely flows past three dimensional wings and the benchmark on the vortex shedding induced by the flow past a squared cylinder [3]. Finally, we discuss the scalability results and the computational efficiency of the proposed solver (implemented in the open-source finite elements library LifeV) in a high performance computing setting. References: [1] Y. Bazilevs, V.M. Calo, J.A. Cottrell, T.J.R. Hughes, A. Reali, and G. Scovazzi. Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows. Computer Methods in Applied Mechanics and Engineering, 197(1-4):173-201, 2007. [2] T.J.R. Hughes, G. Scovazzi, and L.P. Franca. Multiscale and stabilized methods. In Encyclopedia of Computational Mechanics, E. Stein, R. de Borst, and T.J.R. Hughes (eds.). John Wiley & Sons, 2004. [3] B. Koobus and C. Farhat. A variational multiscale method for the large eddy simulation of compressible turbulent flows on unstructured meshes - application to vortex shedding. Computer Methods in Applied Mechanics and Engineering, 193 (15-16):1367-1383, 2003.

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Title: Mesoscale Simulations Investigating the Effects of Shock Wave Stability in Granular Materials with Peridynamics

Author(s): John Foster, Rezwanur Rahman, *UT Austin*; Amanda Peterson, *UTSA*; Tracy Vogler, *Sandia Nat'l. Lab.*.

Research efforts have been undertaken in recent years to investigate the dynamic behavior of granular materials. Many of the investigations have been experimental in nature, consisting of several rounds of Kolsky bar tests on sand with varying moisture content and confining pressures as well as traditional and pressure-shear plate impact. More recently, a set of experiments originally performed in the 60's by Sakharov et al. on the stability of shock waves are being revisited in the context of granular materials . In order to investigate the mesoscale physics that affect the bulk response observed in experiments, we have undertaken a computational simulation effort. The simulations are conducted using a massively parallel computational peridynamics code capable of modeling many thousand individual grains at high resolution resulting in simulations that consist of several million degrees of freedom. Individual intragranular fracture and discrete contact with friction are modeled explicitly in the simulations. Thus, these simulations treat aspects of the problem that were not represented well in previous mesoscale simulations with Eulerian hydrocodes. A discussion of the effects of fracture and friction on force chain formation and bulk wave propagation, and the amplitude decay of perturbed waves in the samples is included.

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Title: Inelasticity and Mixed-Mode Fracture in Porous Rock

Author(s): Craig Foster, Mohammad Hosein Motamedi, David Weed, *U. Illinois, Chicago*.

Failure in porous geomaterials, including rocks, concrete, and soils, is a complex process that can take many forms. At low confining pressures, limited amounts of shear-dilatant plasticity may precede fracture or shear banding in the material. At higher confining pressures, more ductile localization may occur, or bulk compaction and diffuse failure. Depending on the overall stress state and propagation patterns, fractures may remain in shear-compression or become tensile. Pore fluid may also affect the response of all of these behaviors. To predict the onset and propagation of fractures in these materials, an accurate model of the bulk mechanical response of the material is essential. In this research, we modify the Sandia Geomodel, adding a tension cap to more accurately capture tensile failure. The model also captures behaviors such as nonlinear pressure dependence, strength differential effect, and Baushinger effect associated with these materials. The model has a compression cap for inelastic compaction at high mean stresses, though this range will not be examined in this study. An implicit return-mapping algorithm in principal relative stress space is used to improve performance, and is modified for improved efficiency and robustness [1]. Fracture propagation is handled using an enhanced strain finite element with an embedded strong discontinuity. The method continuously tracks fractures as they propagate from element to element using a local tracking algorithm. Opening and sliding along the fractures are determined using a damage-like traction-displacement relationship that accounts for frictional sliding under normal compressive stress and mixed-mode opening and shear displacement under tension. The model is applied to experiments in rock that exhibit both closed fractures with frictional sliding and open fractures. In some cases, initial shear fracture can change orientation as they propagate, so that some fractures may exhibit both sliding and opening at different locations along their length. Time permitting, the presence of pore fluid flow will be added to the fracture model. [1] M. Hosein Motamedi and Craig D. Foster “An improved implicit numerical integration of a non-associated, three-invariant cap plasticity model with mixed isotropic-kinematic hardening for geomaterials“. International Journal of Numerical and Analytical Methods in Geomechanics. In press.

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Title: Non-Linear Mechanics and Cooperative Buckling in Nematic Semiflexible Gels

Author(s): Louis C Foucard, Jordan K Price, William S Klug, Alex J Levine, *UCLA*.

We investigate the effect of geometric non-linearities on the mechanical response of nematic networks of semiflexible filaments. We find that the angle between the nematic director and the direction of shear has a pronounced effect on the nonlinear elastic behavior of anisotropic networks. A combination of numerical simulations and analytic calculations shows that the broken rotational symmetry of the filament orientational distribution leads to a dramatic nonlinear softening of the network at very small strain (on the order of 0.1%). We argue that one can understand this softening in terms of Euler buckling---i.e., the loss of further load-carrying capacity in filaments under compression within the network. With increasing shear strain, this source of geometric nonlinearity appears in the network in a form of heterogenous nucleation in particularly fragile regions (that may be identified by a linear stability analysis), which then grow into ``buckling scars'' that eventually overtake the system. We develop a simple mean-field model for the nonlinear mechanics of such networks and suggest applications of these ideas to a variety of fiber networks and biopolymer systems.

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Title: Resolving the Evolution of Pore Structures in 304-L Laser Welds

Author(s): James Foulk III, Michael Veilleux, John Emery, Jonathan Madison, Helena Jin, Alejandro Mota, Jakob Ostien, *Sandia Nat'l. Lab.*.

The failure of partial-penetration Nd:YAG laser welds in 304-L stainless steel have been investigated through the direct incorporation of pore structures at the specimen level. Micro-computed tomography is employed to characterize multiple weld schedules and develop idealized 3D representations of the size, shape, and spacing of the pores. Pore growth and the subsequent necking are natural outcomes of the simulation. The large deformations between pores require a robust mapping scheme for the remeshing and mapping of internal state variables [1]. We employ higher-order tetrahedral elements to resolve strong gradients and ease the burden of discretizing complex and evolving pore structures. Through our ability to idealize, resolve, and evolve pore structures, we can investigate the performance of candidate weld schedules. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. [1] A. Mota, W. Sun, J.T. Ostien, J.W. Foulk III, and K.N. Long. Computational Mechanics 52, 6 (2013).

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Title: A Phase-Field Approach to Fracture for Mortar Contact Problems

Author(s): Marlon Franke, Christian Hesch, *Karlsruhe Inst. Tech.*.

We aim at a monolithically coupled phase-field model for contact analysis with crack propagation in finite deformations. In particular, a state of the art mortar approach is employed which ensures a precise and smooth stress transition of the contacting bodies, whereas crack propagation is incorporated using a suitable phase-field approach. Within this talk the combination of both is proposed introducing a general framework for finite deformations. For the spatial discretisation standard finite element approximation as well as actual developments of Isogeometric Analysis (IGA) are taken into account. Regarding the phase-field approach for simulation of fracture, second and fourth order phase-field approaches are used (see [1,2]). The former requires C0 continuity, whereas the latter one requires C1 continuity of the approximation space. Moreover, we introduce a multiplicative split of the principal stretches to ensure an anisotropic behavior of the mechanical system, separating tension from compression states (see [3]), leading to a highly non-linear system to be solved. Nowadays, variational consistent mortar based approaches are often used within the context of large deformation contact problems, which can be applied to both the Lagrangian discretisation as well as for the discretisation in the context of IGA. For the latter we use quadratic Non-Uniform Rational B-Splines (NURBS) shape functions and linear shape functions for the Lagrange multiplier field, leading to a simplified and fast mortar framework. In order to reduce the computational effort, taking the locality of both physical events (contact and crack propagation) into account, we introduce a hierarchical refinement scheme for the higher-order IGA approach. This concept relies on a subdivision methodology of the spline basis functions, maintaining the predefined continuity, which is a necessary prerequisite for the application to higher-order phase-field models. [1] Borden, M.J., Hughes, T.J.R., Landis, C.M. and Verhoosel C.V. A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework, Comput. Meth. Appl. Mech. Engrg., 273, 100-118, 2014. [2] Hesch, C. and Weinberg K. Thermodynamically consistent algorithms for a finite-deformation phase-field approach to fracture, Int. J. Numer. Meth. Engng., 99, 906-924, 2014. [3] Hesch, C., Schuss, S., Dittmann, M., Franke, M. and Weinberg, K. Isogeometric analysis and hierarchical refinement for higher-order phase-field models, Journal of Computational Physics, submitted, 2015.

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Scale Tuning of the Non-Linear Dynamics of Tensegrity Metamaterials

Author(s): Fernando Fraternali, Ada Amendola, Gerardo Carpentieri, *U. Salerno*; Robert E. Skelton, Vitali F. Nesterenko, *UC San Diego*.

Engineered foams, cellular solids, granular materials and other acoustic metamaterials have garnered much recent attention in relation to the study of their unique properties, which are not typically found in nature. It has been shown that such structures support vibrational band gaps in the linear dynamic regime (high precompression), and energy transport through solitary waves. The present work deals with a novel application of tensegrity structures as tunable acoustic metamaterials. We show that multiscale chains alternating tensegrity prisms and lumped masses exhibit mechanical response gradually varying from softening to hardening, depending on mechanical, geometrical and local/global prestress parameters [1,2] The dynamics of hardening tensegrity lattices supports extremely compact solitary waves, especially when tensegrity metamaterials are traversed by supersonic compression waves [3]. The “atomic scale localization” of such solitary waves can be employed to create acoustic lenses capable of focusing pressure waves in very compact regions in space, and for nondestructive evaluation and monitoring of materials and structures. Differently, soft tensegrity lattices subject to initial precompression can be employed to construct physical realizations of acoustic metamaterials supporting rarefaction waves [3]. We show that softening tensegrity metamaterials impacted by compression pulses with varying impact velocities are able to convert the impact pulse into a sequence of oscillatory (compression-rarefaction) pulses, which are preceded by a leading solitary rarefaction pulse. Such an interesting behavior can be exploited to design innovative shock absorption devices, and a new class of multiscale metamaterials, to be suitably tuned in terms of local and global prestress. REFERENCES [1] A. Amendola, G. Carpentieri, M. de Oliveira, R.E. Skelton, and F. Fraternali, “Experimental investigation of the softening-stiffening response of tensegrity prisms under compressive loading”, Compos. Struct., 117, 234-243 (2014), doi: 10.1016/j.compstruct.2014.06.022. [2] F. Fraternali, G. Carpentieri, and A. Amendola, “On the mechanical modeling of the extreme softening/stiffening response of axially loaded tensegrity prisms”, J. Mech. Phys. Solids, 74, 136-157, (2015), doi: 10.1016/j.jmps.2014.10.010. [3] F. Fraternali, G. Carpentieri, A. Amendola, R.E. Skelton and V.F. Nesterenko, “Multiscale tunability of solitary wave dynamics in tensegrity metamaterials”, Appl. Phys. Lett., 105, 201903, (2014), doi: 10.1063/1.4902071.

13th U.S. National Congress on Computational Mechanics
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Title: Higher-Order Accurate Integration of Three-Dimensional Geometries Defined by Level-Sets

Author(s): Thomas-Peter Fries, *Graz U. Tech.*.

A unified strategy for the higher-order accurate integration of implicitly defined geometries is proposed. The geometry is represented by a higher-order level-set function. The task is to either integrate on the zero-level set or in the sub-domains defined by the sign of the level-set function. In three dimensions, this is either an integration on a surface or inside a volume. The classical approach is to sub-divide elements recursively until a large number of very fine polygonal sub-elements is achieved [1]. Herein, we propose the use of higher-order, curved sub-elements for the integration. A recursive refinement is only employed in typically less than 1% of the elements. Thereby, the number of integration points is largely reduced without loss of accuracy. Starting point is the identification and meshing of the zero-level set by means of higher-order interface elements. A tailored Newton-Raphson algorithm is used which locates the root of the level-set function along specified straight paths in order to place element nodes. Different variants of search directions are investigated and their important influence on the resulting accuracy of the interface elements is shown. For the volume integration, based on the blending function method [2], special sub-elements are proposed where the element faces coincide with the identified interface elements on the zero-level set. The employed integration rules in the sub-elements have to consider the characteristics of the implied mapping such that consistent integration points are obtained with the ability to integrate polynomials exactly over elements cut by the zero-level set. Numerical results are achieved for the integration of two- and three-dimensional geometries. Systematic convergence studies show the important aspects that influence the accuracy of the quadrature. The resulting integration points may, for example, be used in fictitious domain methods [1] and extended finite element methods [3]. For the case of hexahedral meshes, parts of the approach may also be seen as a higher-order marching cubes algorithm. [1] Abedian, A.; Parvizian, J.; Düster, A.; Khademyzadeh, H.; Rank, E.: Performance of different integration schemes in facing discontinuities in the Finite Cell Method. International Journal of Computational Methods, 10, 2013. [2] Gordon, W.J.; Hall, C.A.: Transfinite element methods: blending function interpolation over arbitrary curved element domains. Numer. Math., 21, 109-129, 1973. [3] Fries, T.P.; Belytschko, T.: The extended/generalized finite element method: An overview of the method and its applications. Internat. J. Numer. Methods Engrg., 84, 253-304, 2010.

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Title: Direct Numerical Simulation of Transport and Mixing in Breaking Internal Waves on Slopes

Author(s): Robert Arthur, Oliver Fringer, *Stanford U.*.

Using direct numerical simulations (DNS), we investigate the turbulent dynamics of breaking internal solitary waves on slopes. A Navier-Stokes code is employed in an idealized, laboratory-scale domain in which an internal solitary wave of depression impinges upon a sloping bottom. The energetics of the flow are analyzed in a volume-integrated sense using the background potential energy framework of Winters et al. [1] while transport is quantified using particle tracking. Peaks in both dissipation and mixing occur during the development of unstable stratification when the wave is breaking [2]. The bulk mixing efficiency, or the overall mixing efficiency of the entire breaking event, is calculated as a function of different incoming wave and slope conditions, and we find that the mixing efficiency is a strong function of a measure of the three-dimensionality of the breaking. Breaking that is characterized by two-dimensional billows is highly efficient, whereas breaking is less efficient when these billows break down and become strongly three-dimensional. Particle tracking shows that onshore transport occurs due to the upslope surge of dense fluid after breaking, while offshore transport occurs due to the intrusion of mixed fluid along the pycnocline [3]. This offshore particle layer resembles an intermediate nepheloid layer, and forms due to irreversible mixing during wave breaking. Cross-shore transport of particles occurs due to turbulence that develops during wave breaking. The lateral transport is quantified with a lateral turbulent diffusivity that is 40 times larger than molecular diffusivity and agrees well with values that would be estimated from a k-ε model. References: [1] Winters, K.B. et al. Available potential energy and mixing in density stratified fluids. J. Fluid Mech. 289:115-128, 1995. [2] Arthur R.S. & Fringer O.B. The dynamics of breaking internal solitary waves on slopes. J. Fluid Mech. 761:360-398, 2014. [3] Arthur R.S. & Fringer O.B. Transport by breaking internal solitary waves on slopes. J. Fluid Mech., submitted.

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Title: Coarse-Grained Molecular Dynamics Simulations of Epoxy Resin During the Curing Process

Author(s): Yao Fu, Jeong-Hoon Song, *U. Colorado-Boulder*; John Michopoulos, *Naval Rsch. Lab.*.

Motivated by the need to establish a multiscale understanding of the mechanical and thermal properties of polymers used for nano-, meso- and macro-composites, we are presenting an investigation of the cross-linking process (associated with curing) of an epoxy phenol novolac and bisphenol-A melt system via coarse-grained molecular dynamics simulations. In particular, we are focusing on the associated structural and physical behaviors of the melts of different cross-linking degree under Couette and Poiseuille flow conditions. At the nanoscale, we also investigated the stress, heat flux and temperature fields that are computable from the quantities of the coarse-grained model of the epoxy resin melt with the extended Hardy's theory to multibody potentials. We have established that the epoxy resin chains tend to reorient along the direction of the imposed Couette flow, and the degree of alignment increases with the cross-linking degree and shear rate. The pronounced reorientation of cross-linked epoxy resin melts can be ascribed to the inter-bonded chains. This conformational change explains the shear thinning behaviors of cross-linked melts that initiate at low shear rates. The cross-linked melts under Poiseuille flow possess less pronounced velocity profiles, accompanied with the smaller temperature rise from the applied gravity force. Due to the size of the nanoscale channel height, the epoxy resin melts under Poiseuille flow can only be approximately predicted via the continuum theory. We have shown that the discrepancies between atomistic simulations and continuum predictions increase as the wall/epoxy interaction strength reduces. This study reveals the variations of important rheological properties during the cross-linking process and elucidates the roles played by the topological changes in the shear flow, thus can contribute to the design and manufacturing of the epoxy-resin based nanocomposites.

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Title: High-Order Shape Functions for Exact Sequence Elements of All Shapes: Part II Pyramids

Author(s): Federico Fuentes, Leszek Demkowicz, Brendan Keith, *UT Austin*.

In 'hybrid meshes', where both tetrahedra and hexahedra are present, pyramids and prisms are fundamental since they act as connecting elements in the mesh. Despite this fact, until recently only first order pyramid elements had been rigorously studied in the four well known energy spaces H1, H(curl), H(div) and L2. This is due to the mathematical requirement of having to use rational polynomials as opposed to the regular polynomials used in the three other elements. This translates to difficulties in defining exact sequence high order FE spaces. Fortunately this issue has been recently tackled, and one set of such spaces was proposed in [1]. However, the shape functions themselves compatible with these spaces (and those of other elements) had never been presented. Such a set of shape functions is presented here for each of the energy spaces. The shape functions are presented in terms of what we call 'pyramid affine coordinates', and moreover they are written in coordinate free format. This allows them to be used with other master element pyramids without any hassles, and even in deformed spaces (e.g. Duffy-transformed cube) where integration is straightforward. The functions have a nice geometrical interpretation and use the same building blocks as those used for the construction of shape functions of other elements. This allows the programming of such shape functions to be greatly simplified. Among other properties, the shape functions are also hierarchical, orientation embedded, and interpolation inequalities are guaranteed for all energy spaces. Additionally, they are also compatible with the typical well-known Nedelec spaces for the other elements, and shape functions for those elements are shown elsewhere. A document showing all this construction and the related proofs relating to traces and conformability is already available in [2]. Moreover, a working code implementing these shape functions is freely available online at [3]. Future work should focus on fast integration of these shape functions and improving the general sparsity and conditioning of the related FE matrices. [1] Nigam, N. and Phillips, J. (2012). High-order conforming finite elements on pyramids. IMA Journal of Numerical Analysis, 32(2):448–483. [2] Fuentes, F., Keith, B., Nagaraj, S., Demkowicz, L. (2015). High Order Orientation Embedded Finite Element (FE) Shape Functions for the Exact Sequence Elements of All Shapes. ICES Reports, UT Austin. [3] The ESEAS library: https://github.com/libESEAS/ESEAS

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Title: Parallel Performance Evaluation of Cache-Cache Elements for Solving Linear Systems

Author(s): Seiji Fujino, *RIIT, Kyushu University*; Kosuke Iwasato, Chiaki Itoh, *Kyushu University*.

We solve efficiently a linear system of equations Ax = b which stem from structural problems and electro-magnetic problems on parallel computers with distributed memory by preconditioned iterative methods. Among many preconditioning technique, Eisenstat-S(Symmetric)SOR is well known to be efficient and robust for the solution of realistic problems. However, the performance of parallel version of E-SSOR does not increase unexpectly because the algorithm of E-SSOR preconditioning includes sequential process in forward and backward substitutions. Moreover, it is underlying to keep mathematical equivalent between some equations appeared in the algorithm of E-SSOR preconditioning. Therefore we devised a new method of Cache-Cache Elements as a parallel technique for Eisenstat-SSOR preconditioning. “Cache-Cache” in French means “hide and seek” in English. We will evaluate and verify parallel performance of Eisenstat-SSOR preconditioned MrsR method (Minimum Residual method with Shadow Residual) for the solution of linear systems with symmetric matrix on parallel computers with distributed memory.

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Title: Numerical Simulation of Seepage-Induced Erosion of Soils by Solving the Darcy/Navier-Stokes Coupled Flows

Author(s): Kazunori Fujisawa, *Kyoto U.*.

The seepage-induced erosion is a major threat to the structures made of earth materials. This paper develops a numerical method to compute and predict the seepage-induced erosion of soils, which is governed by the solid-fluid interaction. To the end, the following three aspects need to be considered: Water flow fields, onset and speed of erosion and boundary tracking between the soil and the water phases. The authors employ the Darcy-Brinkman equations in order to compute the water flow fields around the soils, which easily enable the simultaneous analysis of the seepage flows in the porous media and the water flows in the fluid domain. The onset and the speed of the seepage-induced erosion is predicted by an empirical formula from the flow velocity and the pressure gradient of the seepage water. The boundary tracking scheme based on the phase-field equation is applied for tracking the soil boundary changing with the erosion. This paper shows the numerical results which reveal that the combination of the above three aspects achieves the stable computation of the seepage-induced erosion.

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Title: Finite Element Method: A Strain-Integral-Based, Non-Local Formulation

Author(s): Paolo Fuschi, Aurora Angela Pisano, Dario De Domenico, *U. Mediterr. Reggio Calabria* .

The widespread application in the engineering fields of the displacement-based finite element method (FEM) is due to the circumstance that it furnishes approximate solutions, at the desired extent, of very complex initial boundary value problems. The reliability of such FE solutions is obviously related to the theoretical treatment of the tackled problem that, in many cases, grounds on variationally consistent formulations proper of classical continuum mechanics approaches. If the mechanical problem cannot be described by classical continuum mechanics theory, the FEM, as well as the underneath theory, exhibit their intrinsic limits. The singular stress field predicted at the sharp crack-tip in a continuum fracture mechanics problem, or the inability of classical continuum mechanics in describing deformation phenomena at nanoscale, or also, wave dispersion, strain softening, concomitant size effects (see e.g.[1]) are, among others, typical examples. The FEM applied in the above cases manifests numerical instability, mesh dependence and other drawbacks. There are several ways to overcome the above limits, see e.g.[2] and references therein. The nonlocal continuum approaches, based on an enrichment of the classical modeling by keeping the hypothesis of continuity but introducing an internal length material scale, are, among others, effective tools. Although from a theoretical point of view many aspects of the subject have been already addressed, some problems remain still open from a computational point of view. Following a nonlocal approach of strain-integral type, the present study promotes a nonlocal finite element method, named NL-FEM, whose variational consistency was given in [3]. The numerical implementation of the NL-FEM is presented by focusing on some computational issues as well as on its ability to solve mechanical problems for which a nonlocal elastic treatment is necessary. The nonlocal operators are provided and the main differences with respect to the classical formulation of the FEM are highlighted, as, for example, the presence of a set of self- and cross-stiffness-element matrices able to describe the mutual (nonlocal) interactions between non adjacent elements. The limits and the potentials of the proposed method are also highlighted by analyzing a few case-studies. [1] Z.P. Bazant, L. Cedolin O.C. Stability of structures: elastic, inelastic, fracture and damage theories, World Scientific Publishing Company Ed. (2010). [2] G.A. Maugin, A.V. Metrikine. Mechanics of Generalized Continua One Hundred Years After the Cosserats. Springer New York (2010). [3] C. Polizzotto, “Nonlocal elasticity and related variational principles”, Int. J. of Solid and Structures, 38, 7359-7380 (2001).

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Title: Discrete and Continuum Modeling of Wave Propagation in Chiral Lattices with Local Resonators

Author(s): Andrea Bacigalupo, *IMT Lucca*; Luigi Gambarotta, *DICCA U. Genoa*.

Periodic acoustic metamaterials designed to get complete sound attenuation for a certain frequency range, namely acoustic wave spectral gap, pose interesting issues concerning their mechanical modelling [1-3]. The present analysis is focused on chiral lattices made up of an array of circular rings connected by ligaments and is devoted to understand the influence of resonators located inside the rings on the band gap structure. To get the essential aspects of the system some simplifying assumptions are put forward. The ligaments are assumed massless, while both the rings and the internal resonators are modelled as rigid. A discrete Lagrangian model having six dofs per node is derived and by a Hamiltonian approach the equations of motion are obtained. Dispersive waves in the periodic micro-structure are analysed in terms of dispersive functions and polarization vectors. The exact acoustic and optical branches are derived for harmonic waves in the discrete model. A further simplified description to obtain a synthetic representation of waves propagation is obtained by assuming an expansion of the generalized displacement field around the node of interest. This allows to get an enriched micropolar equivalent continuum whose equations of motion (partially relies on that obtained in [4,5] involves six degree of freedom. To assess the validity limits of the enriched micropolar continuum model the dispersive functions in terms of the fundamental parameters of the mass-in-mass dynamic system are compared with those obtained from the discrete Lagrangian model. References [1] H.H. Huang, C.T. Sun. Wave attenuation mechanism in an acoustic metamaterial with negative effective mass density. New Journal of Physiscs, 11 (2009), 013003-1. [2] D. Bigoni, S. Guenneau, A.B. Movchan, M. Brun. Elastic metamaterials with inertial locally resonant structures: Application to lensing and localization. Physical Review, B 87 (2013), 174303. [3] K.F. Tee, A. Spadoni, F. Scarpa, M. Ruzzene. Wave propagation in auxetic tetrachiral honeycombs. J. of Vibration and Acoustics ASME, 132 (2012), 031007-1/8. [4] A. Bacigalupo, L. Gambarotta. Homogenization of periodic hexa- and tetra-chiral cellular solids. Composite Structures, 116 (2014), 461-476. [5] A. Bacigalupo, L. Gambarotta. A micropolar model for the analysis of dispersive waves in chiral mass-in-mass lattices. Fracture and Structural Integrity, 29 (2014), 1-8.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Organic Thin Films: Evaporation, Phase-Separation and Substrate-Patterning Using Diffuse Interface Models

Author(s): Baskar Ganapathysubramanian, *Iowa State U.*; Olga Wodo, *U. Buffalo*.

Solvent-based thin-film deposition technologies are the most common techniques to fabricate organic thin film, because of their ease to scale-up for large commercial production. All solution-processing techniques involve preparing dilute solutions of two materials in a volatile solvent. After some form of coating onto a substrate, the thin film forms, solvent evaporates leading to phase separation between the two components. We develop a predictive computational framework to model morphology evolution during solvent-based fabrication of thin films. We focus on three distinct physical phenomena: evaporation, phase separation, and substrate-patterning. We naturally formulate this multi-physics problem using a phase field approach using a set of three phase field variables to represent the volume fraction of solvent, and the two solutes that determine the final morphology. We detail the challenges faced in numerically solving this set of equations. A primary challenge is related to the multiple temporal and spatial scales inherent in this transient non-linear problem. By focusing on the two sources of multiple temporal and spatial scales -- one determined by phase separation, and the other driven by the dynamics of evaporation -- we leverage adaptive space-time strategies to efficiently resolve the system evolution. We address several numerical challenges and show how a computationally efficient approach augments experiments and provides predictions at levels close to device scale. We present results for three dimensional problems obtained using a massively parallel version of our solver. We analyze morphology for various process and system variables (such as evaporation rate, substrate effect, blend ratio, solvent type) searching for morphology with desired properties for given application, e.g. organic photovoltaics.

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Title: Performance of Horizontal Fracture in Low-Permeability Shallow Reservoirs

Author(s): Da Peng Gao, Ji Gen Ye, Lei Huang, *PetroChina*.

Low permeability reservoirs become the main potential gradually in the late high water-cut oilfield. For the waterflooding development process of shallow low permeability reservoir after hydraulically fracturing, it is necessary to take into account of both the horizontal fracture and threshold pressure gradient effects on performance of five-spots well pattern. Horizontal fracture is taken equivalent into the elliptical cylinder with reservoir thickness using the equivalent permeability model, and then upon the elliptic seepage theory, the seepage field of a vertical well with horizontal fracture is divided into two parts: radial flow from external formation to equivalent area of horizontal fracture and elliptic flow in the equivalent area of horizontal fracture. The loss of pressure caused by threshold pressure gradient, material balance within the reservoir and multi-well pressure superposition principle are synthesized to calculate the performance of waterflooding. Non-waterflooded independent low permeability reservoir in Xing Shugang oilfield is taken as an practical case, and its oil production, water cut and recovery level of five-spots well pattern with horizontal fracture are analyzed using the performance model.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling the Effects of Stress State on Plastic Deformation and Ductile Damage

Author(s): Xiaosheng Gao, *U. Akron*.

Engineering structures often experience plastic deformation before fracture. The J2-flow theory, which assumes hydrostatic stress as well as the third invariant of the stress deviator has no effect on plastic yielding, has dominated the metal plasticity research for over 100 years. However, increasing experimental evidences have shown that the classical J2 plasticity theory cannot correctly describe the plastic response of many materials. Our recent studies on a variety of structural alloys result in a general form of plasticity model for isotropic materials, where the yield function and the flow potential are expressed as functions of the first invariant of the stress tensor and the second and third invariants of the deviatoric stress tensor. As for ductile fracture, it is well recognized that a main mechanism is due to microvoid nucleation, growth and coalescence. Our recent studies demonstrate that both stress triaxiality and the Lode angle have significant effects on the ductile fracture process. Consequently a modification to the famous Gurson-Tverggard-Needleman porous plasticity model is made to overcome its inability to predict ductile failure under low stress triaxiality, shear dominated conditions. This is done by coupling two damage parameters, representing the volumetric damage (void volume fraction) and the shear damage, respectively, into the yield function and flow potential. The effectiveness of the new model is illustrated through a series of numerical tests comparing its performance with existing models. The new model is shown to be able to predict fracture initiation and propagation in various specimens experiencing a wide range of stress states (including negative triaxialities).

13th U.S. National Congress on Computational Mechanics
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Title: Isoparametric Closure Elements in Boundary Element Method

Author(s): Xiao-Wei Gao, *Dalian U. Tech.*.

An innovation method is proposed for constructing isoparametric elements for closed or semi-closed surfaces. These elements are named "isoparametric closure elements" and not only can well simulate the geometries with spherical, elliptic, and other shaped surfaces, but also can interpolate physical quantitites defined over these surfaces. As a result, these closed surfaces can be discretized into only one closure element along the circumferential direction. A number of closure elements having nodes from 4 to 26 are investigated to examine computational errors and three are recommended to use in the boundary element method (BEM) analysis. These closure elements are applied in BEM for analyzing heat conduction and solid mechanics problems. A technique for eliminating singularities involved in boundary integrals over closure elements is also presented. A number of numerical examples will be given to demonstrate the computational accuracy and efficiency in using the proposed closure elements. Key words: Isoparametric closure element, circle element, spherical surface element, ellipsoid element, boundary element method, element sub-division method.

13th U.S. National Congress on Computational Mechanics
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Title: Model-Order Reduction Of Dynamic Simulation Of Flexible Beams Undergoing Large Rotations

Author(s): Amar Gaonkar, Salil Kulkarni, *Indian Int. Tech. Bombay*.

The finite element modeling of flexible beam problems results in highly nonlinear equations. To obtain a reasonably accurate finite element model of the flexible beam, the number of degrees of freedom required can be large. This results in high computational effort for the solution of such systems. To mitigate such computational difficulties, model order reduction techniques can be employed. In the present work, the full finite element model is first generated using Crisfield's co-rotational approach [1]. The equations of motion are derived using linear interpolation function for axial displacement and cubic interpolation function for transverse displacement. This yields an inertia vector which is a function of both position and velocity, and an internal force vector which is a function of position. The resulting equations of motion are highly nonlinear. To obtain computationally efficient solution of such systems, two different model order reduction approaches are discussed and their performances are compared. In the first approach, a trajectory piecewise linear method [2] is applied to such flexible systems. In this method, a nonlinear system of ordinary differential equations is represented by weighted combination of reduced linear system of equations. In the present work, these reduced linear models are obtained using second order Krylov subspace technique at each linearization point. In the second approach, reduced nonlinear system of equations is obtained using a hybrid method which is based on proper orthogonal decomposition (POD) [3]. The hybrid method is a combination of POD and a two level spatial discretization. The performance of reduced order models generated using both the methods is compared using variety of problems subjected to different loading and boundary conditions. The performance is measured in terms of accuracy, computational efficiency and applicability of reduced order models for different input conditions. References: [1] M. Crisfield. Non-linear finite element analysis of solids and structures, Wiley:New York, 1991. [2] M. Rewienski and J. White., A Trajectory Piecewise-Linear Approach to Model Order Reduction and Fast Simulation of Nonlinear Circuits and Micromachined Devices. IEEE T. Comput. Aid. D, vol 22 155-170, 2003. [3] Krysl,P. and Lall,S. and Marsden,J. Dimensional model reduction in non-linear finite element dynamics of solids and structures, Int J Numer Meth Engg, vol 51 479-504 2001.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Computational Modeling and Stability Analysis for Fluid-Structure Interaction Problems with Applications to Biological and Engineering Systems

Author(s): Sonia Garcia, *US Naval Academy*; Edward Swim, *Sam Houston State U.*; Padmanabhan Seshaiyer, *George Mason U.*.

Multi-physics problems involving Fluid-Structure Interactions (FSI) arise naturally in several engineering and medical applications. Some examples include the biomechanics of intracranial saccular aneurysms coupled with blood flow or the dynamics of flexible wings of micro-air vehicles. Modeling and analysis of such coupled FSI problems is often challenging because of the structure's complicated geometry, material heterogeneity, nonlinear behavior under finite strains and the associated fluid-structure interaction problem. Direct numerical simulation of the associated non-linear equations, governing even the most simplified model depends on the convergence of iterative solvers which in turn rely heavily on the properties of the coupled system. In this talk, we will present a computational solution methodology for solving such coupled FSI problems efficiently using finite element methods. Stability and convergence estimates will also be presented along with computational results that suggest that the technique presented is robust and is a reliable candidate for solving FSI problems.

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Title: Patterning and Growth in Developmental Biology

Author(s): Krishna Garikipati, Gregory Teichert, *U. Michigan*; Alain Goriely, Derek Moulton, *U. Oxford*.

We consider the two main approaches to modelling in developmental biology. The first is patterning, which uses diffusion-reaction equations to establish profiles of morphogens from which cells take cues to differentiate, grow or cease growing, or even to undergo apoptosis. We will make some observations on the regulation of these processes by classical diffusion-reaction equations. The second approach is non-uniform growth-induced folding, rippling and creasing, which is understood to drive morphological development in a wide range of organisms and biological systems. Broad observations will be made, and paths for continued studies will be discussed.

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Title: Coupling Reduced Basis Methods and the Landweber Method to Solve Inverse Problems with a High-Dimensional Parameter Space

Author(s): Dominik Garmatter, Bastian Harrach, Bernard Haasdonk, *U. Stuttgart*.

Solving inverse problems via iterative regularization methods requires many (time-consuming) solutions of the underlying parametrized partial differential equation. One way to speed up the solution process of inverse problems therefore is to reduce the computational time of the forward solution, e.g. via the reduced basis method. The reduced basis method is a model order reduction technique which constructs a low-dimensional subspace of the solution space. Galerkin projection onto that space allows for an approximative solution. An efficient offline/online decomposition enables the rapid computation of the approximative solution for many different parameters. The simple and intuitive approach of weaving reduced basis methods into the solution process of inverse problems is the substitution of the forward solution by a global reduced basis approximation in a given regularization algorithm. The limitations of this approach in the context of a PDE with a high-dimensional parameter space will be shortly discussed in this talk. The main topic of the talk is a new method that combines the ideas of the reduced basis method with the Landweber method and is inspired by [1]. The general idea is to construct a reduced basis space tailored around a given inverse problem instead of constructing a global reduced basis space providing a good approximative solution for every parameter in the parameter space (like it is normally the case in reduced basis methods). This will be done in an adaptive procedure: the inverse problem will be solved up to a certain degree with a Landweber method that is projected onto the current reduced basis space. The method then utilizes the resulting parameter to enrich the reduced basis space. This iteration is made until the whole inverse problem is solved. First numerical results will demonstrate the method. [1] V. Druskin and M. Zaslavsky. On combining model reduction and Gauss–Newton algorithms for inverse partial differential equation problems. Inverse Problems, 23(4):1599, 2007.

13th U.S. National Congress on Computational Mechanics
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Title: Adaptive FEM in the Approximation of Clusters of Eigenvalues of the Laplace Problem in Mixed Form

Author(s): Lucia Gastaldi, *U. Brescia*.

In this talk we consider the finite element discretization of eigenvalues and eigenfunctions arising from elliptic partial differential equations. We review briefly a priori and a posteriori error estimates [1-2] and discuss how the theory applies to the case of multiple eigenvalues [3]. It turns out that, in the adaptive finite element approximation of eigenvalues and eigenfunctions arising from partial differential equations, it is necessary to take into account not only multiple eigenvalues but also clusters of them, because the eigenvalues of interest and their multiplicities may not be resolved by the initial mesh [4]. In this spirit we consider the discretization of elliptic partial differential equations in mixed form by means of Raviart-Thomas or Brezzi-Douglas-Marini families of finite elements and present a result obtained recently in collaboration with D. Boffi, D. Gallistl, and F. Gardini, where it is proved the optimal convergence of the adaptive scheme for the approximation of clusters of eigenvalues. REFERENCES [1] D. Boffi, “Finite element approximation of eigenvalue problems”, Acta Numer., 19, 1-120 (2010). [2] D. Boffi, F. Gardini, L. Gastaldi, “Some remarks on eigenvalue approximation by finite elements”, in Frontiers in Numerical Analsis – Durham 2010, Springer lecture notes in Computational Science and Engineering, 85, 1-77 (2012). [3] D. Boffi, L. Gastaldi, “Some remarks on finite element approximation of multiple eigenvalues”, Appl. Numer. Math., 79, 18-28 (2014). [4] D. Gallistl, “Adaptive nonconforming finite element approximation of eigenvalue clusters”, Comput. Methods Appl. Math., 14, 509-535 (2014).

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Title: Reduced Rank Preconditioners

Author(s): Paolo Gatto, Jan Hesthaven, *EPFL*.

Schur complements that arise from finite elements discretizations of certain differential problems, e.g., elliptic PDE's, are amenable to fast linear algebra techniques. Those usually include probabilistic algorithms that construct an approxiamate matrix decomposition within linear complexity. Furthermore, the decomposition is such that the approximate inverse can be applied within linear complexity as well. Although those ideas are the working horse of fast direct solvers, they are seldom used for building preconditioners for iterative solvers. In this talk I illustrate the construction of such preconditioners and discuss preliminary results of their effectiveness for problems other than elliptic, e.g., hyperbolic problems and coupled problems that result in a compact perturbation of an isomorphism.

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Title: Electronic Structure Study of an Edge Dislocation in Aluminum

Author(s): Mrinal Iyer, Vikram Gavini, *U. Michigan*; Balachandran Radhakrishnan, *UC San Diego*.

This talk presents a real-space formulation of orbital-free density functional theory using finite-element basis to study the defect-core and energetics of an edge dislocation in Aluminum. Our study shows that the core-size of a perfect edge dislocation is around ten times the magnitude of the Burgers vector. This finding is contrary to the widely accepted notion that continuum descriptions of dislocation energetics are accurate beyond 1-3 Burgers vector from the dislocation line. Consistent with prior electronic-structure studies, we find that the perfect edge dislocation dissociates into two Shockley partials with a partial separation distance of 12.8 Angstroms. Interestingly, our study revealed a significant influence of macroscopic deformations on the core-energy of Shockley partials. We show that this dependence of the core-energy on macroscopic deformations results in an additional force on dislocations, beyond the Peach-Koehler force, that is proportional to strain gradients. Further, we demonstrate that this force from core-effects can be significant and can play an important role in governing the dislocation behavior in regions of inhomogeneous deformations.

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Title: Finite Element Methods for Free- and Moving-Boundary Problems Using Universal Meshes

Author(s): Evan Gawlik, Adrian Lew, *Stanford U.*.

We present a class of high-order finite element methods for the solution of free- and moving-boundary problems. The methods make use of a universal mesh: a background mesh that contains the moving domain for all times and conforms to its geometry at all times by perturbing a small number of nodes in the neighborhood of the moving boundary. The methods are able to handle large domain deformations easily (a common difficulty faced by conventional deforming-mesh methods) while representing the geometry of the moving domain exactly (a challenging task for conventional fixed-mesh methods). We then introduce a unified analytical framework for establishing the convergence properties of a wide class of numerical methods for moving-boundary problems with prescribed boundary evolution. This class includes, as special cases, the technique described above as well as conventional arbitrary Lagrangian-Eulerian (ALE) schemes. We present applications to problems involving fluid-membrane interaction, phase-changes, and flow past moving obstacles.

13th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization for Additive Manufacturing: Incorporating Printer Capabilities to Reduce Post-Processing and Maximize Performance

Author(s): Andrew Gaynor, James Guest, *Johns Hopkins U.*.

Additive manufacturing (AM) drastically expands the design freedoms over traditional manufacturing methods. These freedoms are not limitless, however, and must be considered when designing a part to be additively manufactured. This work considers various additive capabilities, including printer resolution, sparse infill design and orientation, and sacrificial support material elimination. Sparse infill is of particular interest since most commercial 3D printers provide you with a choice in infill patterning and orientation, however there is no connection between the infill characteristics and the part performance. Also of concern is the need for post-print support material removal, typically achieved through dissolving in the case of polymer-based Fused Deposition Modeling (FDM), or through manual removal in the case of Selective Laser Melting (SLM) and Stereolithography (SLA) type methods. This work proposes to exploit the maximum printable overhang angle, so that parts may be printed without requiring support material. Overall, the design paradigm for this work is to integrate AM capabilities into the topology optimization algorithm so that the engineer can fully exploit each AM technology. Through this work, not only are current topology optimization capabilities connected to AM processes, but also new topology optimization algorithms are developed to incorporate AM specific constraints into the design methodology. First, a relatively straightforward connection is made between minimum length scale control (minimum feature size) and achievable printing resolution. Minimum feature size control is imposed through the projection based Heaviside Projection Method (HPM). Secondly, expanding on the projection-based methods, an algorithm is proposed to design for the patterning and orientation of sparse infill. This approach, unlike current standard practice, incorporates loading and boundary conditions to rigorously optimize infill of parts originally designed for solid fill. Finally, a new topology optimization algorithm is proposed to eliminate the need for sacrificial support material through design, exploiting the maximum achievable overhang angle for each AM technology. This algorithm is formulated through a modification to the typical topology optimization formulation to include an additional projection scheme in which the overhang constraint is imposed. In this way, the overhang constraint is naturally achieved in a similar fashion to the Heaviside Projection Method (HPM) for minimum length scale control: without explicit constraints. The proposed algorithms are tested on standard design problems and preliminary results show excellent agreement with the imposed constraints. As one might expect in the case of the overhang constraint design algorithm, the optimized designs clearly depend on the specified build direction.

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Title: New Closed-Form Analytical Solutions to Some Classical Problems in Elastodynamics

Author(s): George Gazonas, *U.S. Army Rsch. Lab.*.

This talk will present new closed-form analytical solutions to some classical wave propagation problems in 1-D, homogeneous, linearly elastic media. We begin with the classical problem of wave propagation in a finite elastic strip subjected to a Heaviside stress loading at one end, with the other end fixed. The solution for this mixed boundary value problem is expressed in terms of an infinite series of Heaviside functions [1]. A new closed-form analytical solution to the finite elastic strip problem can be expressed in terms of the floor (or greatest integer) function. The floor function construct is used ubiquitously in mathematical programming and number theory. Next, we review the classic problem of a transiently displaced string [2], given by f(t) at x = 0, with the end x = l allowed to slide freely along a line perpendicular to the undeformed string. Courant and Hilbert [2] plot the infinite Heaviside series solution for the special case where the imposed displacement is a unit amplitude pulse of duration ■ starting at t = 0; our new solution to this problem is explicit and expressed in terms of floor functions. Interestingly, Courant and Hilbert [2] state that even though the solution is written in terms of an infinite sum that: "…for every instant t, only a finite number of terms are different from zero." This remark cultivated the idea that a closed-form solution might be obtained for this class of problems. Finally, a 1-D impact problem is presented in which a semi-infinite flyer collides with the front face of a stationary target plate of finite thickness. The back face of the target is bonded to another semi-infinite medium. Explicit expressions for the stress and velocity in the target are given in terms of floor functions for all times after impact. It is shown that the asymptotic (long-time) stress and velocity in the target is independent of the target's elastic properties. These solutions are exact, and thus form an important contribution to benchmark problems [3] in use for verification of large-scale computational codes. [1] Eringen, A.C.; Suhubi, E.S. Elastodynamics, Volume II, Linear Theory, Academic Press, New York, 1975. [2] Courant, R.; Hilbert, D. Methods of Mathematical Physics, Volume II, Partial Differential Equations, Interscience Publishers, New York, 1962. [3] Idesman, A.; Samajder; H., Aulisa, E.; Seshaiyer, P. Benchmark problems for wave propagation in elastic materials, Comput. Mech., 43(6), 797–814, 2009.

13th U.S. National Congress on Computational Mechanics
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Title: Patient-Specific Cardiac Dynamics and Predictive Modeling for Cardiac Assist Device Engineering

Author(s): Michael W. Gee, Marc Hirschvogel, *TU München*; Stephen N. Wildhirt, *AdjuCor GmbH*.

The adequate predictive modeling of cardiac mechanics, that is capable of accurately reproducing the heart's functionality and response to external disturbances, remains a challenging task. Especially the various physical phenomena involved, i.e. structural and fluid mechanics as well as electrophysiology, pose high demands on the numerical solution strategies. We present a high-resolution 3D nonlinear finite element model based on patient-specific heart geometries, which includes an active material law prescribing the ventricular contraction along a generic muscle fiber orientation [1]. In addition, a passive material model captures the highly anisotropic nonlinear behavior of the myocardium [2]. Furthermore, the structural model is strongly coupled with the ventricular blood compartments, addressed through 0D models to represent valve functionality and the circulatory system. We use a closed-loop lumped-parameter model which is able of modeling veinous return by assuring conservation of volume within the loop, similar to [4] and [5]. This leads to a monolithic windkessel-structural system of equations being solved within an iterative Newton-Raphson scheme with adequate block preconditioners at hand and allows for the physiologically meaningful solution of the heart contraction mechanics without considering a full fluid-structure interaction problem. We demonstrate efficient strategies for calibrating the model to real-life experimental data. Given a calibrated patient-specififc heart model that reproduces a specific situation of heart failure, we demonstrate the model's predictability for cardiac assist device engineering and optimization. "[1] Nagler, A.; Bertoglio, C.; Gee, M.W.; Wall, W.A. Personalization of cardiac fiber orientations from image data using the Unscented Kalman Filter. Functional Imaging and Modeling of the Heart, Lecture Notes in Computer Science, 7945, 132-140, 2013. [2] Holzapfel, G.A.; Ogden, R.W. Constitutive modelling of passive myocardium: a structurally based framework for material characterization. Phil. Trans. R. Soc. A, 367, 3445-3475, 2009. [3] Westerhof, N.; Lankhaar, J.-W.; Westerhof, B.E. The arterial windkessel. Med. Biol. Eng. Comput., 47 (2), 131-141, 2009. [4] Blanco, P.J.; Feijo, R.A. A 3D-1D-0D computational model for the entire cardiovascular system. Computational Methods in Hemodynamics, XXIX (59), 5887-5911, 2010. [5] Sainte-Marie, J.; Chapelle, D.; Cimrman, R.; Sorine, M. Modeling and estimation of the cardiac electromechanical activity. Computers and Structures, 84, 1743-1759, 2006.

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Title: Influence of Microplasticity in Metal Foams on Macroscopic Damping Behavior

Author(s): Maximilin Geissendoerfer, Carsten Proppe, *Karlsruhe Inst. Tech.*.

Metal foams are developed and produced due to their distinctive properties like low stiffness to density ratio, chemical reactions or energy absorption. Another characteristic property is the damping capacity of foams which is significantly higher compared to a sample made by dense material. The damping capacity depends on both internal factors like microstructure of the foam or the material itself and external factors like loading frequency, loading amplitude and temperature. The interaction and influence of all these factors on damping is still a big challenge in research. A series of experimental studies on damping exists already, e.g. [1]. Our research is focused on developing a computational model which predicts the influence of microscopic damping mechanisms on macroscopic dynamic behavior. Hereby damping because of the existence of microplastic zones is investigated. Due to the characteristic microstructure of open-cell metal foams, local plastic yielding occurs while the foam is still macroscopically linear elastic. This results in local energy dissipation which can be described by a damping parameter. A linear elastic foam model [2] has been further developed which includes microplasticity. For non-representative volume elements the distribution function of a homogenized damping parameter is calculated. The homogenized damping parameter is discretized and projected on the macro scale by using Karhunen-Loeve-decomposition [3]. It also takes the amplitude-dependency of the damping into account. In final case studies the influence of the calculated damping parameter and its distribution function on the dynamic behavior of beams and plates will be presented. References [1] Golovin I.S., Sinning H.-R.: Damping in some cellular metallic materials, Journal of Alloys and Compounds 355 (2003) 2-9 [2] Geißendörfer M., Liebscher A., Proppe C., Redenbach C., Schwarzer D.: Stochastic multiscale modeling of metal foams, Probabilistic Engineering Mechanics 37 (2014) 132-137, doi:10.1016/j.probengmech.2014.06.006 [3] Phoon, K.K., Huang S.P., Quek S.T.: Implementation of Karhunen-Loeve expansion for simulation using a wavelet-Galerkin scheme, Probabilistic Engineering Mechanics 17 (2002) 293-303

13th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification of Reacting Multi-Phase Flow Simulations Towards Scale-Up and Rapid Development of Industrial Size Advanced Clean Coal Technologies

Author(s): Aytekin GEL, *ALPEMI Consulting, LLC*; Mehrdad Shahnam, Jordan Musser, *Nat'l. Energy Tech. Lab.*; Aun K. Subramaniyan, *GE Global Rsch. Center*; Jean-François Dietiker, *West Virginia U. Rsch. Corp.*.

The U.S. Department of Energy has great interest in technologies that will lead to reducing the CO2 emission of fossil fuel burning power plants. Integrated Gasification Combined Cycle (IGCC) power plants can potentially capture and store streams of CO2, reducing the impact of power generation on our atmosphere. In an IGCC power plant, a gasifier converts coal into synthesis gas, which is used to generate electricity in a gas turbine. Advanced modeling and simulation capabilities have the promise of significantly reducing the time and cost of the development and deployment of technological processes such as gasification. Modeling and simulation allows rapid scale-up of prototype technologies, reducing or even potentially avoiding costly intermediate scale-up testing. In practice, the credibility of simulation tools needs to be established with uncertainty quantification (UQ) methods. The goal of this project has been to explore the applicability of available UQ techniques and open source toolboxes in assessing uncertainties in gasification simulations. In the first phase of this initiative, non-intrusive UQ methods such as parametric input uncertainty propagation through sampling of a deterministic computational fluid dynamics (CFD) model of a fluidized bed gasifier was employed. In the second phase, Bayesian calibration and UQ methods were employed for the same gasifier configuration where extensive experimental data was available. Our talk will be presenting our preliminary findings for the initial phase of this initiative in which a surrogate model was constructed and an UQ analysis through the forward propagation of input parameters was performed without any calibration. For this purpose, an Optimal Latin Hypercube sampling approach was employed to construct an adequate surrogate model for investigating the effect of uncertainty in 3 key design parameters (coal flow rate, coal particle diameter and steam to oxygen ratio) on several quantities of interest (such as CO, CO2, H2 species mole fractions at the exit). Deterministic simulations of the gasifier with both an open-source CFD code developed at NETL and a commercial CFD code were carried out. By nature, reacting transient multiphase flow simulations are inherently complex and computationally expensive, which makes sampling methodology and sample size critical components in the overall UQ assessment. We will also present our experiences and some of the challenges encountered in implementing a conceptual UQ framework to employ open source UQ engines and toolboxes (in particular PSUADE, GPM/SA and DAKOTA) integrated with our CFD solver through a workflow protocol.

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Title: 3D Image-Based Workflows for Model & Mesh Generation in Biomechanics Simulations: The Latest Trends and Applications

Author(s): Kerim Genc, *Simpleware Inc*.

3D image-based Finite Element (FE) model generation techniques enable robust simulations to be obtained from 3D scans (MRI, CT, micro-CT etc.) for a range of both research and commercial applications in the life sciences. These applications include medical device design (implants, stents, etc.), and simulations of anatomical processes or interactions between the human body and consumer products such as helmets, diapers, footwear etc. More recently, 3D Image-based modelling & mesh generation has also gained a strong momentum in a number of CAD/CFD simulation workflows in new application areas such as reverse engineering, non-destructive evaluation (NDE), materials research and rapid prototyping, all of which also have significant benefits for biomechanics applications. We will provide an overview of the development of and recent advances in image-based model and mesh generation for simulation, including how techniques complement but also offer advantages over traditional computer-aided design (CAD) meshing. A particular benefit over CAD methods is the ability to mesh multiple domains that have conforming interfaces where two or more structures meet, eliminating the need for manual re-meshing before simulation. Attention will be paid to the different ways in which 3D images (voxels) can be meshed, including the generation of volumetric meshes directly from greyscale data, as well as surface reconstruction approaches and techniques for refining mesh density and defining material properties. Discussion will be made of the flexibility possible with mesh generation tools for obtaining robust and reliable results that take into account partial volume effects and preserve image topology and volume. We will go on to discuss how image-based simulation models and meshes are used for various types of FEA and CFD simulations. Examples will be given of how meshing techniques can be combined with other modelling workflows, such as statistical analysis, as well as how image-based meshes can be integrated with CAD objects. Recent case studies will be provided of how image-based meshing is being used for biomechanical and other applications, and suggestions made of how techniques can be adapted to more powerful imaging and simulation technologies. Key contributions offered by this paper include the presentation of cutting-edge methodologies for 3D image processing and 3D image-based mesh generation, as well as discussion of recent ‘real-world’ applications and what they mean for the future development of 3D images based modelling in biomechanics and related areas.

13th U.S. National Congress on Computational Mechanics
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Title: A Cell-Centered Finite Volume Method for Solving Multi-Dimensional Hyperelasticity Equations Written Under Total Lagrangian Form

Author(s): Gabriel Georges, Jérôme Breil, Pierre-Henri Maire, *Bordeaux U.*.

Finite Volume discretization of non-linear elasticity equations seems to be a promising alternative to the traditional Finite Element discretizations currently employed [Bonet et al., A first order hyperbolic framework for large strain computational solid dynamics. Part I: Total Lagrangian isothermal elasticity, Comput. Methods Appl. Mech. Engrg. 283 (2015) 689-732]. In this work, we intend to derive a Finite Volume discretization to compute the large deformations of elastic isotropic isothermal materials including shock waves. The materials under consideration are characterized by an hyperelastic constitutive law for which the second Piola Kirchhoff stress tensor is the derivative of a strain energy function with respect to the right Cauchy Green tensor. In this manner, the material model satisfies the principle of material frame indifference and is thermodynamically consistent. The set of governing equations consists of the linear momentum equation, which is written under total Lagrangian form, and the geometric conservation law (GCL), which is nothing but the time rate of change of the deformation gradient. Extending the methodology described in [Vilar et al., A discontinuous Galerkin discretization for solving the two-dimensional gas dynamics equations written under total Lagrangian formulation on general unstructured grids, Journal of Computational Physics, 276 (2014) 188-234] for Lagrangian gas dynamics, we present a nominally second-order cell-centered discretization for solving the equations of non-linear elasticity on tetrahedral grids. This work can also be viewed as an extension of the two-dimensional first-order scheme introduced in [Kluth et al., Discretization of hyperelasticity on unstructured mesh with a cell-centered Lagrangian scheme, Journal of Computational Physics, 229 (2010) 9092-9118]. We provide a spatial discretization of the deformation gradient for which the Piola compatibility condition is satisfied. Further, the numerical fluxes at cell interfaces are approximated to ensure a thermodynamic-like dissipation inequality. The robustness and the accuracy of this Finite Volume method for non-linear elasticity are assessed by means of numerous representative test cases.

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Title: The Influence of Dynamic Rollover Test System (DRoTS) Constraints on Vehicle Response

Author(s): Bronislaw Gepner, Matthew Panzer, Qi Zhang, Jason Kerrigan, *U. Virginia*.

Rollover type accidents account for less than 5% of passenger vehicle crashes, but claim more than a third of occupant fatalities. The regulatory agencies have tried to protect the vehicle passengers by introducing rollover safety regulations such as Federal Motor Vehicle Safety Standard (FMVSS) 216. However, the efficacy of FMVSS 216 is often questioned, due to the quasi-static characteristic of the prescribed load and the acceptance criterion of maximum roof resistance force. An alternative test procedure is available through the use of a Dynamic Rollover Test System (DRoTS), a laboratory-based test apparatus capable of simulating the dynamic conditions of a vehicle in a rollover accident (Kerrigan et al., 2011). DRoTS allows for the vehicle roll, pitch, roll-rate and vertical and lateral motion (via a movable roadbed) while constraining longitudinal translation and vehicle yaw. Thus, the design of DRoTS reduces the degrees of freedom and initial conditions of the vehicle from 9 to 5. Since DRoTS is intended to mimic real-world vehicle rollover conditions, the question arises whether the reduced and constrained degrees of freedom have a significant effect on the test outcome. The goal of this study is to identify whether the imposition of the constraints or the reduction of initial parameters inflicts a significant difference in vehicle deformation response. A LS-DYNA finite element (FE) model of a mid-sized crossover sport-utility vehicle was used to compare the effect of the reduced degrees of freedom and reduced initial conditions outcome of rollover. The vehicle model was validated using results of the experimental DRoTS test on the same vehicle. A sensitivity study was done using touchdown conditions extracted from 12 different rollover events identified in a national crash database (CIREN). DRoTS constraints were assessed using all 12 rollover simulations by comparing the vehicle deformation response between the constrained and unconstrained conditions. The reduction of the input parameters was evaluated through the full factorial combination of reduced input parameters for all 12 cases (192 rollover simulations). The results show that the effect of the constraints imposed by DRoTS is minimal. The mean relative difference of vehicle deformation was below 5%, which is below the variation from test to test. Adversely, the reduction of input parameters shows a large variation in the vehicle response. All of the reduced input parameters had a significant influence onto the outcome of the rollover, with vehicle yaw having the greatest effect between the DRoTS and real-world results.

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Title: Efficient Computing of the Phase-Field Model of (Brittle) Fracture Using the Monolithic Scheme and Adaptive Mesh Refinements

Author(s): Tymofiy Gerasimov, Laura De Lorenzis, *Technische U. Braunschweig*.

The phase-field approach for modeling fracture phenomena in elastic solids is a very promising framework which has gained popularity within the last decade, see the review paper [1] and the references therein. In practice, already a two-dimensional quasi-static phase-field formulation is computationally quite demanding: (i) the need to resolve the small length scale calls for extremely fine meshes, at least locally, in a crack phase-field transition zone, (ii) due to non-convexity of the free-energy functional, a robust, but a priori non-efficient staggered solution scheme based on algorithmic decoupling is typically used, e.g. in [2,3,4]. We discuss an efficient (i.e. fast and accurate) strategy for quasi-static phase-field computing of (herein, brittle) fracture, using a monolithic solution scheme and adaptive (error-controlled) mesh refinement strategy [5]. [1] M. Ambati, T. Gerasimov, L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. Computational Mechanics, 55, 383-405, 2015 [2] B. Bourdin, G.A. Francfort, J.J.Marigo. The variational approach to fracture. Journal of Elasticity, 91, 5-148, 2008 [3] C. Kuhn, R. Müller. A continuum phase field model for fracture. Engineering Fracture Mechanics, 77, 3625-3634, 2010 [4] C. Miehe, M. Hofacker, F. Welschinger. A phase field model for rate-independent crack propagation: robust algorithmic implementation based on operator splits. Computer Methods in Applied Mechanical Engineering, 199, 2765-2778, 2010 [5] T. Gerasimov, L. De Lorenzis. Fast and reliable computing of the phase-field model of (brittle) fracture using the monolithic scheme and adaptive mesh refinement, in preparation

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Title: Inverse Problem of Electrocardiography From a Multiphysics Perspective

Author(s): Cesare Corrado, *King's College London*; Jean-Frederic Gerbeau, *INRIA-UPMC*; Philippe Moireau, *INRIA*.

This presentation addresses the inverse problem of electrocardiography from a new perspective, by combining electrical and mechanical measurements. Our strategy, proposed in [1], relies on a model of the electromechanical contraction which is registered on ECG data [2] but also on measured mechanical displacements of the heart tissue typically extracted from medical images. In this respect, we establish the convergence of a sequential estimator which combines for such coupled problems various state of the art sequential data assimilation methods in an efficient framework [3]. We aggregate a Luenberger observer for the mechanical state and a Reduced Order Unscented Kalman Filter applied on the parameters to be identified, and a POD projection of the electrical state. Then using synthetic data we show the benefits of our approach for the estimation of the electrical state of the ventricles along the heart beat compared with more classical strategies which only consider an electrophysiological model with ECG measurements. Our numerical results actually show that the mechanical measurements improve the identifiability of the electrical problem allowing to reconstruct the electrical state of the coupled system more precisely. Therefore, this work is intended to be a first proof of concept, with theoretical justifications and numerical investigations, of the advantage of using available multi-modal observations for the estimation and identification of an electromechanical model of the heart. [1] Identification of weakly coupled multiphysics problems. Application to the inverse problem of electrocardiography Cesare Corrado, Jean-Frederic Gerbeau, Philippe Moireau Journal of Computational Physics, Elsevier, 283, pp.271-298, 2015 [2] Mathematical modeling of electrocardiograms: a numerical study, Muriel Boulakia, Serge Cazeau, Miguel Fernández, Jean-Frederic Gerbeau, Nejib Zemzemi Annals of biomedical engineering, 38 (3), 1071-1097, 2010. [3] Joint state and parameter estimation for distributed mechanical systems, Philippe Moireau, Dominique Chapelle, Patrick Le Tallec Computer methods in applied mechanics and engineering, 197 (6), 659-677, 2008.

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Title: Interface Control Domain Decomposition Method

Author(s): Marco Discacciati, *UPC*; Paola Gervasio, *U. degli Studi di Brescia*; Alfio Quarteroni, *EPFL*.

Interface Control Domain Decomposition (ICDD) is a novel method designed to address partial differential equations (PDEs) by overlapping subdomains. Interface controls are unknown functions used as Dirichlet boundary data on the interfaces of an overlapping decomposition designed for solving a given boundary value problems. The control variables are computed through an optimal control problem with interface observation ([1], [2], [3]). When the ICDD method is applied to classical (homogeneous) elliptic equations, it can be regarded as (yet) another domain decomposition method to solve elliptic problems ([1]). However, what makes it interesting, are its convergence properties of grid independence, its robustness with respect to the possible variation of operator coefficients, and the possibility to use non-matching grids and non-conforming discretizations inside different subdomains. In particular, if hp-FEM (or spectral element methods (SEM)) are used, both the mesh size h and the polynomial degree p can be conveniently chosen independently in each subdomain without affecting the convergence rate of ICDD. The evaluation of the jump between the state solutions across the interfaces (the boundaries of the overlapping regions) can be performed by an interpolation step with a computational cost that does not affect the global efficiency of the method. In particular, no mortar approach is needed to guarantee the optimal convergence with respect to the discretization parameters. ICDD methods become especially attractive when applied to solve heterogeneous PDEs, that is coupled problems where different kinds of PDE are set up in different subdomains. A noticeable example is in multiphysics applications, in which case the different PDEs are designed to model different kinds of physics. In particular we consider the coupling between surface and subsurface flows, modeled e.g. by Stokes and Darcy equations. In this case, the minimization problem set on the interface control variables, that is enforced by ICDD method, can in principle assure the correct matching between the two different physics without requiring the a-priori determination of the transmission conditions at the interface between them ([2],[3]). [1] Discacciati M, Gervasio P, Quarteroni A (2013) The Interface Control Domain Decomposition (ICDD) Method for Elliptic Problems. SIAM J. Control Optim 51 (5): 3434-3458. [2] Discacciati M, Gervasio P, Quarteroni A (2014) Interface Control Domain Decomposition (ICDD) Methods for Heterogeneous Problems. Int. J. Numer. Meth. Fluids 76: 471-496. [3] Discacciati M, Gervasio P, Quarteroni A (2014) Interface Control Domain Decomposition (ICDD) Method for Stokes Darcy coupling. Technical report no. 22/2014 MATHICSE-EPFL.

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Title: Analysis of Damage in Anisotropic Media with a New Peridynamic Material Model

Author(s): Mazdak Ghajari, Lorenzo Iannucci, *Imperial College London*; Paul Curtis, *Defence Sci. & Tech. Lab.*.

Prediction of crack initiation and propagation in anisotropic media, such as composites, ceramics, rocks and bones, is of great technological and medical importance. To deal with this problem, researchers have proposed extensions to current numerical methods, such as the Finite Element Method (FEM), the Boundary Element Method and the extended FEM. These methods are all based on the classical elasticity theory, which includes spatial derivatives. Silling [1] has proposed a new formulation of the elasticity theory, called the peridynamic theory, in which spatial derivatives are replaced with integrals. As a result, in peridynamics, the equations can be easily evaluated where there is discontinuity in the displacement field, in contrast to the classical elasticity theory. In this paper, a new material model within the framework of the bond-based peridynamics has been presented [2]. This model extends the capabilities of the theory to predict complex fracture phenomena, e.g. spontaneous crack nucleation and crack branching, curving and arrest in anisotropic media. The spherical harmonic expansion is employed to define the dependencies of the parameters of the bond-based theory, e.g. the bond stiffness constant and the critical stretch, on bond orientation. As a result, these parameters are continuous functions of bond orientation in the principal material axes. This model is appropriate for fracture analysis of anisotropic material with random orientation, such as polycrystalline microstructures. The model was used to simulate crack propagation in a cortical bone compact tension specimen [2]. Very good agreement was found between the experimental and predicted crack initiation loads and crack paths. The capabilities of the model were further demonstrated by estimating the macroscopic elastic properties of a polycrystalline aggregate, which was in good agreement with experimental data, and predicting intergranular and transgranular fracture in the microstructure. References [1] S. A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. Journal of the Mechanics and Physics of Solids, 48(1), 175-209, 2000. [2] M. Ghajari, L. Iannucci, P. Curtis. A Peridynamic material model for the analysis of dynamic crack propagation in orthotropic media. Computer Methods in Applied Mechanics and Engineering. 276, 431-452, 2014.

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Title: Effect of Uniformly Distributed Tangential Follower Force on Stability of Rotating Flexible Cantilever Pipe Conveying Fluid

Author(s): Amir Karimi Nobandegani, Esmaeal Ghavanloo, S. Ahmad Fazelzadeh, *Shiraz U.*.

The problem of structural stability in non-conservative systems has been attracted many attentions in engineering science and a huge amount of work has been done in this field. Rotating cantilever pipes are found in several practical engineering applications. Moreover, the fluid flowing inside the pipe acts as the concentrated tangential follower force at the tip of the pipe, and exerts a lot of influences on the dynamic behavior of a pipe. Therefore, a large number of papers have presented about the dynamic behavior of fluid conveying pipes since the early 1960s. In addition to the effect of fluid flowing inside the pipe, the uniformly distributed tangential follower force on the pipes is also an important parameter. It should be noted that there is no existing model so far in the literature able to take into account the combined effects of the fluid flowing inside the pipe, uniformly distributed tangential follower force and rotation of pipes. For reliable and practical design of these structures, it is necessary to estimate the modal characteristics accurately. Therefore, it is highly desirable to find and utilize simple and accurate methods. In this paper, dynamic behaviors of cantilever pipe rotating in a horizontal plane, conveying fluid and uniformly distributed tangential follower force are studied. The Euler–Bernoulli beam theory is used as structural model of the pipe. The Hamilton's principle is used to derive the equation of motion and boundary conditions of the system. Using the Galerkin method, the obtained partial differential equation is transformed to ordinary differential equations. The eigenfunctions of a cantilever beam which satisfy the prescribed geometric boundary conditions are used as basis functions in the Galerkin method. The equation of motion is expressed in matrix form and is solved numerically using the Runge-Kutta method. The influences of the design parameters such as the rotating angular velocity, the velocity of fluid flow and magnitude of uniformly distributed tangential follower force are elucidated by the numerical simulation. The results are also compared with those reported in the literature.

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Title: Non-Linear, Size-Dependent Buckling and Post-Buckling Dynamics of Microbeams

Author(s): Mergen Ghayesh, *U. Wollongong*; Hamed Farokhi, *McGill U.*.

This paper aims at analysing the three-dimensional buckling and post-buckling dynamics of perfect and imperfect Timoshenko microbeams subject to mechanical and thermal loads. The equations of motion for the longitudinal, transverse, and rotational motions are derived via use of Hamilton's principle as well as the modified couple stress theory. These three coupled nonlinear partial differential equations are reduced via Galerkin's technique, yielding a set of ordinary differential equations with coupled nonlinear terms. The resultant equations are solved by means of the pseudo-arclength continuation technique as well as an eigenvalue analysis. As the temperature is increased, for the geometrically perfect microbeam in the absence of the transverse load, the stability is lost by a super-critical pitchfork bifurcation at the critical temperature, leading to a static divergence (buckling); the post-buckling state is obtained and resonant response over it, due to a mechanical transverse force, is analyzed. For the initially imperfect microbeam, as the temperature is increased, the initial curvature amplitude increases with no instabilities; the resonant response of the system over the new deflected configuration is obtained. The effect of different parameters on the nonlinear dynamics and stability of the system is studied.

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Title: A Multi-Scale Approach to Modeling Intergranular Fracture Process in Metallic Alloys

Author(s): Benyamin Gholami Bazehhour, Kiran N. Solanki, Jay Oswald, *Arizona State U.*.

In this study, we investigate the development of a hierarchically-driven multiscale algorithm for finite element analysis of intergranular fracture process in metallic microstructures. A two-dimensional framework for non-linear extended finite element method (XFEM) is developed in which the mesh is not required to be conformal to the topology. XFEM provides benefits over conventional finite element method simulations, especially in three-dimensional simulations, in terms of computational costs. Necessary tools for simulation of fracture process are developed for this purpose. Grain boundary properties are quantified by atomistic simulations and employed in the XFEM framework using a modified cohesive zone model to bridge the different length scales. A rate-dependent crystal plasticity model is incorporated into XFEM to account for orientation dependent elasto-plastic deformation. Effect of different microstructural properties on the crack initiation and growth is studied.

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Title: Challenges for Exascale Scalability of Elliptic Solvers Using a Model Poisson Solver and Comparing State-of-the-Art Methods

Author(s): Amir Gholaminejad, Georg Biros, *UT Austin*.

According to DOE's office of science, one of the challenges for exascale scalability is the need for new programming paradigms and numerical methods that can effectively use the unprecedented computational powers of near future. In this talk, we consider a Poisson problem as a model and compare the state-of-the art, massively parallel numerical solvers. We study the Fast Fourier Transform (FFT), the Fast Multipole Method (FMM), the Geometric MultiGrid method (GMG), and Algebraic MultiGrid method (AMG). In particular, we present weak and strong scaling results as well time to solution for uniform and adaptive grids, using the current systems. The tests are performed on the Stampede system at the Texas Advanced Computing Center and on the Titan system at the Oak Ridge National Laboratory. In the largest test case, we consider a Poisson problem with 600 billion unknowns on 229,379 cores of Titan. The results show that FFT is the fastest method for smooth source functions with uniform grid, while FMM and GMG are the method of choice for source functions with highly localized features.

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Title: Mechanical Behavior of Wooden Members of Historic Buildings Strengthened by FRP Composites

Author(s): Yaghob Gholipour, *U. Tehran*.

Wood is one of the most important materials used in historic buildings with cultural value around the world. The wooden members of historical buildings are often damaged and need to be strengthened. Because of importance of the cultural and heritage value, they must be reinforced without considerable apparent damage. Fiber reinforced plastic (FRP) could be a suitable material for this reason. This research investigates the mechanical behavior of old wood members strengthened by glass fiber reinforced Plastic (GFRP) and carbon fiber reinforced Plastic (CFRP) composite sheets. The advantages of this material lie in low density, high tensile strength and corrosion resistance. In this research more than 90 specimens were cut of wooden elements of some actually damaged historical buildings. The specimens divided into two sets that both of them were prepared and tested according to D143-06 specification of ASTM standard in different configurations. As reinforcement material two types of unidirectional FRP sheets, Carbon Fiber Reinforced Plastic (CFRP) and Glass Fiber Reinforced Plastic (GFRP) were used to strengthen corresponding specimens. The bonding adhesive meets ASTM 2559 and ANSI A190.1 criteria. They were reinforced with various layers of FRP sheets and bundle conditions. A three-point bending test procedure was used to simulate the beam response under gradual load. The ultimate strength, modulus of elasticity, bonding and the mode of failures were investigated. The wood members strengthened by GFRP and CFRP show considerable improvement on the mechanical properties. The specimens strengthened by CFRP show higher flexural strength in comparison with the similar specimens reinforced by GFRP but the second is more advantageous for appearance.
Keywords: Historic Building, Composite Materials, Wood Structures, Fiber Reinforced Plastic

13th U.S. National Congress on Computational Mechanics
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Title: Micromechanical Modeling of the Elastoplastic Behavior of a Carbonated Petroleum Cement Paste

Author(s): Hamid Ghorbanbeigi, *U. Lille 1*.

The contact of carbon dioxide (CO2) with the cement paste used in oil wells causes carbonation of the cement pastes hydrates. This chemical reaction leads to the formation of calcite grains which consequently reduces the porosity. These changes of the microstructure, affect the mechanical property of the cement paste. An experimental campaign was first carried out, where multiaxial mechanical tests were realized under temperature (90 degree C) on a petroleum cement paste called ``G'' class cement (Takla et al. 2010) to get close to the borehole conditions. The study characterized the effects of carbonation on the mechanical properties of sound, partially and fully carbonated samples. These results were then used to develop a micro-macro model. The validation of the micro-macro model was realized, assuming an average for the porosity and the calcite formed during carbonation of the samples, in order to consider them homogeneous throughout the carbonation process. The aim of the current study is to make a more realistic approach by considering the samples becoming heterogeneous during carbonation. For this purpose, finite element calculations are necessary. The samples are meshed with an acceptable number of elements to be able to make calculations for a heterogeneous structure with a sound core and a carbonated circular area from the outer part of the cylindrical samples. Using this technique it is aimed to be able to predict the elastoplastic behavior of a partially carbonated cement paste.

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Title: Coupled Fluid-Chemical Computational Modeling of Anticoagulation Therapies in a Stented Artery

Author(s): Anirban Ghosh, Rajat Mittal, *Johns Hopkins U.*.

Coronary artery disease (CAD) is the most common form of heart disease and the leading cause of death worldwide. One common method of treating coronary artery disease is through balloon angioplasty and placement of stents in the stenosed artery. A relatively rare but serious complication that can result from this process is stent thrombosis, the formation of clots due to vascular wall damage by the stent. Stent thrombosis been associated with 30-day mortality rates of 10-25%, and can occur days to even years following stent placement. [1] The common treatment for stent thrombosis is to provide patients with anticoagulant and antiplatelet therapy through the bloodstream. However, this treatment increases the risk of bleeding disorders, not only limited to the stented artery but also including gastrointestinal and intracranial bleeding. A study found that 3.1% of patients receiving antiplatelet therapy suffered bleeding complications over a 28-month period. [2] The present study compares this method of delivering anticoagulant to the arterial wall through the bloodstream with a local delivery method via a drug-eluting stent. In this study the flow in the artery and the biochemical processes of the coagulation cascade, platelet activation, and platelet aggregation are modeled in two dimensions. A computational fluid dynamics model is developed that couples an incompressible flow solver with a convection-diffusion-reaction equation. The flow solver uses a sharp-interface immersed boundary method to characterize pulsatile flow over the curved wires of the stent. The convection-diffusion-reaction equations are solved for the 16 coupled reactions that make up the coagulation cascade, as well as reaction and transport equations for both active and inactive platelet species. The results find that the drug-eluting stent delivery of anticoagulant is more effective in reducing platelet activation and clotting, while also providing a more localized anticoagulant distribution. [1] Kirtane AJ, Stone GW. How to minimize stent thrombosis. Circulation 2011;124:1283–7. [2] Berger PB, Bhatt DL, Fuster V, Steg PG, Fox KA, Shao M, Brennan DM, Hacke W, Montalescot G, Steinhubl SR, Topol EJ. Bleeding complications with dual antiplatelet therapy among patients with stable vascular disease or risk factors for vascular disease: results from the Clopidogrel for High Atherothrombotic Risk and Ischemic Stabilization, Management, and Avoidance (CHARISMA) trial. Circulation. 2010; 121:2575-2583.

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Title: Distribution-Enhanced Homogenization Framework and Model for Heterogeneous Elasto-Plastic Problems

Author(s): Somnath Ghosh, Coleman Alleman, *Johns Hopkins U.*; Curt Bronkhorst, DJ Luscher, *Los Alamos Nat'l. Lab.*.

Multi-scale models are powerful computational tools for simulating heterogeneous materials, offering a tractable means to model sufficiently large spatial domains. The ability of these models to resolve material behavior at different scales and communicate across them is fostering unprecedented advances in modeling. Within the framework of computational multi-spatial scale analyses, hierarchical models enable unidirectional transfer of information from lower to higher scales, usually in the form of effective material properties. Analytical models have been developed, e.g. for linear elasticity, but microscale solutions are known analytically for a limited class of problems. To obtain solutions for realistic microstructures, explicit forms for the macroscale constitutive relations can be developed from homogenization of the microscopic response. This requires determination of functional forms for the macroscale constitutive parameters with respect to the microstructure, referred to as parametric homogenization. The macroscale constitutive models represent the effect of morphological features and evolving microstructural mechanisms through homogenized parameters and volume averages of the underlying microscale fields. Typically, parametric homogenization takes the functional forms of the microscale constitutive relations and uses similar or identical functional forms. This is successful because the macroscale constitutive behavior is usually well-approximated by some homogeneous medium, but there is currently no general way to derive a new set of macroscale constitutive relations that more accurately represents the microscale behavior, if necessary. This paper proposes a new alternative approach, the distribution-enhanced homogenization framework (DEHF), where the macroscale constitutive relations are formulated in a series expansion based on the microscale constitutive relations and moments of arbitrary order of the microscale field variables. This approach allows for improved accuracy in representing the microscale fields through their distributions; increasing the order of the truncated series expansion results in increasing fidelity of the macroscale approximation of the microscale constitutive behavior. Here, some examples are presented in which the macroscale DEHF model is able to capture the microscale response of the material without any reparametrization of the microscale constitutive relations for use at the macroscale. In these examples, the higher-order moments of the mechanical fields are written in terms of the evolving first moments of the mechanical fields and static moments related to the microscale geometry or morphology. While these closed form expressions will not be available in all circumstances, the traditional techniques, e.g., parametric homogenization, could be used to determine these relationships for a general case.

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Title: An Error in Constitutive Equations Approach for Elasticity Imaging Using Ultrasound Data

Author(s): Susanta Ghosh, Manuel Diaz, Zilong Zou, Mark Palmeri, Wilkins Aquino, *Duke U.*; Mahdi Bayat, Mostafa Fatemi, *Mayo Clinic*.

Elasticity and viscoelasticity imaging techniques are of high relevance in medicine as mechanical properties of soft tissues are well-known predictors of the onset and progression of disease. These techniques have been intensely investigated due to their promise, for instance, in the detection of breast cancer, cardiovascular disease, and liver disease, among others. Ultrasound-based elasticity imaging modalities are very attractive due to their low-cost and portability. However, computational inverse problem approaches face several major challenges when ultrasound data is used: uni-directionality of measured displacements, planar acquisitions, lack of boundary information, and noise, among others. In this talk, we will present our current progress in developing computational inverse problem techniques that effectively address these challenges. To this end, we have developed a PDE-constrained optimization approach based on the minimization of an error in constitutive equations functional augmented with a least squares data misfit term. Through variational arguments, we demonstrate that the current framework allows naturally for problems in which boundary conditions are partially or completely unknown, making it a very suitable candidate for ultrasound-based elasticity imaging. We will present inversion results using both simulated and experimental ultrasound data. In our synthetic data cases, finite element computations were polluted using noise that emulates the ultrasound-tracking process. We will also present reconstructions obtained from laboratory phantoms in which bulk waves were excited using the radiation force of ultrasound and tracking of the propagating waves was performed using the same ultrasound transducer. Our results indicate that our proposed framework could be effectively coupled current ultrasound imaging devises to produce accurate reconstructions of mechanical fields. Furthermore, our results highlight the potential of our approach to be employed in clinical settings.

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Title: Characteristic-Based Flux Splitting for Implicit-Explicit Time Integration of Low-Mach Number Flows

Author(s): Debojyoti Ghosh, Emil Constantinescu, *Argonne Nat'l. Lab.*.

Low-Mach number flows, such as atmospheric flows, are characterized by two different time scales corresponding to the flow velocity and the acoustic waves. The stability limit of explicit time integration methods is restricted by the speed of sound; however, the acoustic waves often do not have a significant impact on the flow phenomenon. Most numerical algorithms for unsteady low-Mach number flows solve the Navier-Stokes equations with the incompressible assumption (where the speed of sound is assumed to be infinite), or use a preconditioned implicit time-integration method to integrate the compressible Navier-Stokes equations. In the context of atmospheric flows, an alternative approach is to eliminate the acoustic mode by using a hydrostatic model. Recently, implicit-explicit time-integration methods were applied to non-hydrostatic atmospheric flows (Giraldo, Restelli, Laeuter, SIAM J. Sci. Comput., 2010, and Giraldo, Kelly, Constantinescu, SIAM J. Sci. Comput., 2013) where a perturbation-based splitting of the hyperbolic flux was used. In this study, we propose a characteristic-based splitting of the convective flux in the Euler/Navier-Stokes equations to separate the velocity and acoustic time scales. The eigen-structure of the flux is used to decompose it into a “slow” flux consisting of the entropy wave propagating at the local flow velocity, and a “fast” flux consisting of the acoustic waves propagating at the relative speed of sound. Additive Runge-Kutta methods are used to integrate the former in time explicitly and the latter implicitly. Thus, the linear stability limit of the algorithm depends on the flow velocity, and not the speed of sound, while maintaining high order accuracy in time. This approach is used in a conservative finite-difference algorithm where the weighted essentially non-oscillatory (WENO) (Jiang, Shu, J. Comput. Phys., 1996) and the compact-reconstruction WENO (Ghosh, Baeder, SIAM J. Sci. Comput., 2012) schemes are used for the spatial discretization. We also propose a linearization of the “fast” flux in time such that the system of equations resulting from semi-implicit time integration can be solved efficiently without compromising the stability limit of the overall algorithm or introducing an error in the discretization. Our proposed approach is verified for several benchmark flow problems where the flow velocities are significantly smaller than the speed of sound. We present results that demonstrate the performance and accuracy of our algorithm.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A New Tensor-Based Decomposition of Spatiotemporal Random Processes

Author(s): Debraj Ghosh, Anup Suryawanshi, *Indian Inst. Sci.*.

Spatiotemporal processes appear in numerous applications such as temperature field, velocity field of fluid, response of vibrating bodies, precipitation. Efficient finite-dimensional decomposition of such process is a challenging task from computational point of view. The Karhunen-Loe`ve (KL) decomposition, which is a popular choice for pure spatial or temporal process, turns out to be very expensive for these processes. A new decomposition for spatiotemporal process is presented here. This is based on tensor decomposition of the covariance, following the analogy of the KL. The temporal variation of the spatial covariance of a spatiotemporal process is first expressed as a third order tensor. In a discrete setting it results in a finite dimensional tensor where the covariance matrix among the spatial locations for a given time instant serves as a slice of the tensor. This tensor is then decomposed as a sum of outer products of vectors using existing methods. Numerically this is implemented using an alternating least squares. These basis vectors, along with a set of basic random variables, are then used to represent the spatiotemporal process. This decomposition is applied to a heat equation and a vibration response. This decomposition is further equipped with data assimilation for wind velocity modeling and is applied to a set of real measured data published in the literature. References: Ghosh D and Suryawanshi A, Approximation of spatio-temporal random processes using tensor decomposition, Communications in Computational Physics, Global Science, Volume 16, Number 1, 75-95, 2014. Suryawanshi A and Ghosh D. Wind speed prediction using spatio-temporal covariance, Natural Hazards, Springer, Volume 75, 1435--1449, 2015.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Orbital Free Density Functional Theory Using Higher-Order-Finite Differences

Author(s): Swarnava Ghosh, Phanish Suryanarayana, *Georgia Inst. Tech.*.

Density functional theory (DFT) is an accurate and widely used theory for describing the quantum-mechanical electronic structure of matter. In this approach, the intractable problem of interacting electrons is simplified to a tractable problem of non-interacting electrons moving in an effective potential. Even with this simplification, DFT remains extremely computationally expensive. In particular, DFT scales cubically with respect to the number of atoms, which restricts the size of systems that can be studied. Orbital free density functional theory (OF-DFT) represents a simplification of DFT applicable to metallic systems that behave like a free-electron gas. Current implementations of OF-DFT employ the plane-wave basis, the global nature of the basis prevents the efficient use of modern high-performance computer architectures. We present a real-space formulation and higher-order finite-difference implementation of periodic Orbital-free Density Functional Theory (OF-DFT). Specifically, utilizing a local reformulation of the electrostatic and kernel terms, we develop a generalized framework suitable for performing OF-DFT simulations with different variants of the electronic kinetic energy. In particular, we develop a self-consistent field (SCF) type fixed-point method for calculations involving linear-response kinetic energy functionals. In doing so, we make the calculation of the electronic ground-state and forces on the nuclei amenable to computations that altogether scale linearly with the number of atoms. We develop a parallel implementation of our method using Portable, Extensible Toolkit for scientific computations (PETSc) suite of data structures and routines. The communication between processors is handled via the Message Passing Interface (MPI). We implement this formulation using the finite-difference discretization, using which we demonstrate that higher-order finite-differences can achieve relatively large convergence rates with respect to mesh-size in both the energies and forces. Additionally, we establish that the fixed-point iteration converges rapidly, and that it can be further accelerated using extrapolation techniques like Anderson’s mixing. We validate the accuracy of our results by comparing the energies and forces with plane-wave methods for selected examples, one of which is the vacancy formation energy in Aluminum. Overall, we demonstrate that the proposed formulation and implementation is an attractive choice for performing OF-DFT calculations.

13th U.S. National Congress on Computational Mechanics
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Title: A Computational Framework for Polyconvex Large Strain Electromechanics

Author(s): Antonio J Gil, Rogelio Ortigosa, Javier Bonet, *Swansea U.*.

The numerical simulation of smart materials is pushing the limits of current computational mechanics techniques. The present work focuses on the simulation of Electro Active Polymers (EAPs). EAPs can be classified into two large groups: Electronic Electroactive Polymers (or field activated) and Ionic Electroactive Polymers. Within the first group, Dielectric Elastomers (DEs) form a very attractive subgroup of polymeric materials, which have drawn the attention of scientists over the last two decades. Their fast dynamic response, large electrically induced deformations and lightness surpass those of the highly rigid piezoelectric polymers. Moreover, the versatility of DEs enables their use in sensor and energy harvesting applications. The initial linearised variational framework developed for rigid ceramics and piezoelectric polymers is no longer applicable for the numerical simulation of these new materials. For instance, a voltage induced area expansion of 1962% in a thin DE film material called 3MTM VHBTM4910 has been recently reported. In this specific case, electro-mechanical instability is harnessed as a means for obtaining these electrically induced massive deformations. Hence, special attention needs to be paid when defining appropriate constitutive laws, since the introduction of non-physical instabilities, such as loss of ellipticity of the model, might lead to a polluted numerical solution. In this paper, appropriate constitutive laws for nonlinear electro-elasticity are proposed based upon the extension of the concept of polyconvexity introduced by Ball [2] for nonlinear elasticity. The new definition of polyconvexity uses an extended set of variables and requires convexity of the internal energy with respect to the entire set. This new electro-kineto variable set leads to new work conjugates and enables the introduction of new interesting Hu-Washizu type [1] of mixed variational principles. For the purpose of numerical simulation, the Finite Element Method is preferred for discretisation. Moreover, and bearing in mind the incompressible nature of DEs, a novel SUPG stabilised Finite Element formulation with linear tetrahedral elements for the interpolation of displacements, electric potential and hydrostatic pressure is presented for the first time in the context of electro-mechanics. Finally, a series of numerical examples are presented in order to assess the capabilities of the new formulation [3]. References [1] J.M. Ball, Convexity conditions and existence theorems in nonlinear elasticity. Archive of Rational Mechanics Analysis, 63, pp. 337-403, 1977. [2] J. Bonet, A.J. Gil, R. Ortigosa. A computational framework for polyconvex large strain elasticity. Computer Methods in Applied Mechanics and Engineering, 238, pp. 1061-1094, 2015. [3] A.J. Gil, R. Ortigosa, J. Bonet. A computational framework for polyconvex large electromechanics. Under review.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: What is a Good Linear Finite Element... On a Generic Polytope?

Author(s): Andrew Gillette, *U. Arizona*; Alexander Rand, *CD-Adapco*.

The notion of what constitutes a "good" linear finite element on geometries other than simplices and cubes remains largely unexplored. We use harmonic coordinates as a means to investigate this question, arriving at a few key conclusions. On convex polygons, harmonic coordinates in general provide no improvement over standard interpolation on the constrained Delaunay triangulation of the polygon. On non-convex polygons, however, harmonic coordinates can provide optimal interpolation estimates even when all triangulations fail to do so. We also present the extension and implication of these results to finite elements on non-convex polyhedra in 3D.

13th U.S. National Congress on Computational Mechanics
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Title: Predicting Shape Effect on Effective Thermo-Mechanical Properties for Heterogeneous Particulate Composites Using Higher-Order Statistical Micromechanics

Author(s): Andrew Gillman, Karel Matouš, *U. Notre Dame*.

Predicting effective transport and mechanical properties of random heterogeneous materials has many scientific and engineering applications including flow in porous rock, deformation of structural composites, and electric current in conductive adhesives, just to name a few. Various mathematical and numerical methods have been utilized to predict the macroscopic response of these materials, but accurate prediction for highly packed configurations of particles with arbitrary particle shape and material contrast ratio has proved elusive. The focus of this work is to estimate the effective material behavior using higher order statistical micromechanics and to develop microstructure-statistics-property relations. In past statistical mircomechanics work, assumptions are often made about the morphology in order to simplify analysis. Moreover, utilizing statistical information beyond two-point statistics has proved elusive due to difficulties in accurately computing higher order correlations. To limit microstructural assumptions, a detailed three-dimensional characterization of the morphology is obtained using micro- computer tomography in conjunction with novel image processing and shape characterization methods. The statistical description of these many particles systems is computed utilizing Monte Carlo-based statistical sampling schemes in a parallel high performance computing (HPC) framework, and this description is utilized within micromechanics theories for predicting the overall material response. In this presentation, we focus on computing third-order estimates of effective thermal conductivity and elastic constants for highly packed polydisperse systems only assuming statistical isotropy. This work relies on parallel adaptive methods rooted in computational mechanics for efficiently representing one-, two-, and three-point probability functions arising in third-order models [1]. The computational methods are rigorously verified for well-studied systems of overlapping and impenetrable spheres, and excellent agreement with simulation data is exhibited. Using the rigorously verified framework, the effective conductivity and elastic moduli are computed for systems composed of crystalline inclusions (Platonic solids) at various particle concentrations [2]. A significant shape effect for the thermal conductivity is predicted, whereas the effective elastic moduli are less sensitive to the morphology. In addition, statistical micromechanics models incorporating imperfect surface behavior are explored. REFERENCES: [1] A. Gillman, K. Matouš, “Third-order model of thermal conductivity for random polydisperse particulate materials using well-resolved statistical descriptions from tomography”, Physics Letters A, 378(41): 3070-3073 (2014). [2] A. Gillman, G. Amadio, K. Matouš, and T. Jackson, “Third-order thermo-mechanical properties for packs of Platonic solids using statistical micromechanics”, submitted to Proceedings of the Royal Society A (2015).

13th U.S. National Congress on Computational Mechanics
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Title: DEM Simulation of the Dry and Weakly Wetted Bulk Flow on a Pelletizing Table

Author(s): Anton Gladkyy, Holger Lieberwirth, Ruediger Schwarze, *TU Bergakademie Freiberg*.

The discrete element method is a modern numerical technique for particle simulations. It is becoming indispensable for industrial applications with granular flow processes are playing an important role. This paper will mainly be focused on bulk material behavior of a pelletizing table. Those tables are used for agglomeration of small particles into larger ball-shaped forms. A weakly wetted model bulk material (glass beads) is agitated on a small-scale pelletizing table with different rotational speeds. Corresponding DEM simulations are performed with the open-source DEM software YADE. The linear viscoelastic model in combination with the capillary bridge models of Willett or Rabinovich/Lambert are used to simulate the wet contacts between two spherical particles [1]. Experimental observations and snapshots from the DEM simulations of the bulk material behavior are in good qualitative agreement in the entire operating regime of the pelletizing table. On the base of particle and contact information provided by DEM, different rotational movement regimes of the particles are identified and correlated to the rotational speed of the pelletizing table. Especially the critical rotational speed, at which the bulk material circulates along the edges of the table, differs significantly from values which are expected from an estimation based on a well-known heuristic equation. Further quantities, such as the total number of contacts, coordination number, force intensity and others are used for a more detailed evaluation of the internal dynamics of the bulk material on the pelletizing table. In summary, it is shown that DEM is able to predict main parameters of bulk flow on the pelletizing table. This information can be used for optimizing the operating modes of technical equipment in various industries. [1] A. Gladkyy and R. Schwarze. Comparison of di■erent capillary bridge models for application in the discrete element method. Granular Matter , 16(6):911-920, 2014.

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Title: Sensitivity Analysis and Post Shot Tuning

Author(s): James Glimm, Jeremy Melvin, Hyunkyung Lim, Verinder Rana, *Stony Brook U.*; Baolian Cheng, David Sharp, *LANL*.

Sensitivity Analysis and Post Shot Tuning J. Glimm, B. Cheng, D. H. Sharp, J. Melvin, H. Lim, V. Rana We address a common problem: a large number of submodels are combined to construct a model of a complex, integrated experiment, with an overall discrepancy. A common strategy is based on post shot tuning, to sort out the sensitive and plausible submodel modifications to yield an improved validation. The weakness is possibile undected cancelling errors. Thus a follow on strategy is detailed examination of the identified submodels and their sensitivities and proposed modifications, conducted in part in idealized situations where V&V/UQ is possible. This time honored approach is examined for Inertial Confinement Fusion experiments with attention to Rayleigh-Taylor and Richtmyer-Meshkov mixing submodels. We consider three submodels, the radiation drive, the cold shell thermodynamics and the turbulent mixing. The first depends on tuned radiation drives, to obtain ageement of the simulated and measured implosion velocities, based on studies of D. Clark. The second builds on a proposal of Cheng et al. to add preheat to the cold shell. The third is based on turbulent mixing. We find a reduction in neutron yield of a factor of 2 from the entropy modeling and a factor of 4 from the turbulence modeling, in combinaion a factor of 8, which nearly brings at least one of the shots modeled into agreement with experiment. However, not all measured parameters are in agreement, and we have cancelling errors. As outlined above, we now consider a refined analysis, and draw upon our background in the modeling of Rayleigh-Taylor and Richtmyer-Meshkov instabilities. Our modeling of Rayleigh-Taylor growth rates yields results usually within error bars, or in the worst case within +/- 5% of them, and is unique in the extent of this type of validation. Extensions to higher reynolds numbers were shown to be a small effect. We determined the significant dependence of map of the space time transport parameters on r and t, for an ICF implosion. This information guides the application of a 1D mix model based on the buoyancy drag equation. Future work will consider 2D and eventually 3D simulations to more accurately analyze the role of mixing in ICF implosions. Separately, we will perform an A-B comparison of our Front Tracking methodology with high quality codes lacking this feature.

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Title: Applying Vessel Inlet/Outlet Conditions to Patient-Specific Models Embedded in Cartesian Grids

Author(s): Aaron M. Goddard, H.S. Udaykumar, Sarah C. Vigmostad, *U. Iowa*.

Cartesian grid flow solvers offer many advantages when used to model cardiovascular flows: complex geometries can be embedded without body-fitted volume meshes, and moving boundaries (such as a valve leaflet or coronary artery moving during the cardiac cycle) are easily implemented without remeshing or added computational time [1]. Our group has developed a parallel and adaptively refined Cartesian approach for application to cardiovascular simulations, particularly to study valve dynamics and other fluid-structure interaction systems [2]. Patient-specific cardiovascular simulations deviate (often significantly) from the orthogonal directions of the Cartesian domain. In many cases this requires the addition of non-physiologic extensions to the vessel. Furthermore, these extensions must be created in a manner as to terminate in a direction normal to the cuboid boundary, such that some degree of artificial curvature is required. To avoid introducing non-physiologic flow patterns as a result, these extensions are created to be sufficiently long such that in the physiologic domain, the flow is not affected, but unfortunately, this can dramatically increase the computational requirements of the simulation [2]. To address these limitations, we will present a recently developed approach in which vessel inlet/outlet boundary conditions can be applied to any segment within the Cartesian grid domain, regardless of orientation or location. To further reduce computation time and memory requirements, we have incorporated the ability to “prune” the domain, another feature of particular value to arteries and other physiologic simulations. Through these new developments, the benefits of Cartesian grid flow solvers can be more widely applied to cardiovascular fluid dynamics simulations, to enable further insight about disease progression and treatment, to be gained from computational modeling. References: 1. Kensuke Yokoi, Feng Xiao , Hao Liu, Kazuaki Fukasaku. Three-dimensional numerical simulation of flows with complex geometries in a regular Cartesian grid and its application to blood flow in cerebral artery with multiple aneurysms. Journal of Compuatational Physics 2005; 202 1:1-19 2. Seth I. Dillard, John A. Mousel, Liza Shrestha, Madhavan L. Raghavan, Sarah C. Vigmostad. From medical images to flow computations without user-generated meshes. International Journal for Numerical Methods in Biomedical Engineering 2014; 30:1057-1083

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Title: Multi-Model Ensemble Assimilation for Reducing Model Errors in Forecasts

Author(s): Humberto C. Godinez, *Los Alamos Nat'l. Lab.*; Sean Elvidge, *U. Birmingham*.

The simulation of complex physical phenomena is commonplace in many areas of physics. As our knowledge of the physical phenomena increases, more complete models can be developed. Nevertheless, model errors and bias, resulting from uncertain parameters and unaccounted physical processes, still have a significant influence on the accuracy of model forecasts. In general, because the true state of a physical system, such as the atmosphere, is highly complex, it remains fundamentally impossible to describe all its processes in any one single model, no matter how complex the model itself is. In this talk we present a multi-model ensemble system [1] coupled with an assimilation algorithm to improve the forecast of the ionosphere-thermosphere environment [2]. The main advantage of our approach is that combining the common fields between a number of models that include different physics and/or approximations can mitigate errors and/or bias suffered by any one model. In order to enhance the model forecast, each model is weighted according to the difference between the model prediction and observed data available. The weighted sum is then utilized in an assimilation algorithm to remove any possible error/bias in any each individual model for the forecast. This approach has the advantage that the forecast will not be worse than the best model, and in many cases, better than any individual model forecast. We present a number of multi-model weighting schemes and their relative performance compared against observational data available. For our particular application, we will use three different models for the ionosphere-thermosphere, and derived neutral density observations from a couple of satellites. A number of numerical experiments are presented which compare the forecast performance of single-model and multi-model assimilation techniques. [1] S. Elvidge, H.C. Godinez, and M.J. Angling, Improved modelling of upper atmospheric densities using multi-model ensembles, 3rd IMA Conference on Mathematics in Defence Proceedings, 2013. [2] C. Tebaldi and R. Knutti, The use of the multi-model ensemble in proba- bilistic climate projections, Phil. Trans. R. Soc. A 365 (2007), 2053–2075.

13th U.S. National Congress on Computational Mechanics
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Title: Thermal Boundary Resistance from Atomic Simulations: Parameterization of a Microstructure Informed Continuum Model

Author(s): Nipun Goel, Edmund Webb, Alparslan Oztekin, Sudhakar Neti, *Lehigh U.*.

Silicon Carbide is a candidate material for high temperature microelectronic applications; as such, it is attractive to consider its use in thermoelectric devices for harvesting waste heat associated with automotive exhaust. However, for SiC to be a viable thermo-electric material for high temperature applications, its thermoelectric figure of merit ZT = S2SigmaT/Kappa must be improved significantly. S is Seebeck coefficient, Sigma is electrical conductivity, and Kappa is thermal conductivity. A strategy that has been extensively explored for improving ZT in materials is to reduce ■ while not affecting ■ by introducing phonon scattering features in the material structure that have minimal effect on electron transport. Thermal boundary, or Kapitza, resistance at microstructure grain boundaries (GB) is one mechanism advanced as being able to hamper phonon transport but not electron transport, partly because the mean free path of phonons in many materials is significantly larger than that of electrons. However, it has been advanced that the Kapitza resistance revealed by, e.g., Molecular Dynamics (MD) simulations in different materials is too low to account for certain experimental observations of thermal conductivity dependence on grain size. Thus, GB impurities have been described as possibly being able to increase Kapitza resistance. This phenomenon is explored here via non-equilibrium MD simulations of β-Silicon Carbide (3C-SiC) to investigate the effect of doping at the GB on the thermal transport across the GB at 1000K. Symmetric tilt GB with a tilt about the [111] plane are explored and the effect of tilt angle (i.e. the degree of misorientation) is explored. For each GB modeled, the role of dopant concentration at the boundary, dopant mass, and dopant/matrix interaction strength are explored. Generally, Kapitza resistance is observed to increase with increasing dopant concentration. At higher dopant/matrix interaction strength, there exists a tendency for dopant atoms to form more layered structures, resulting in less significant increases in Kapitza resistance. At low interaction strength, clustered dopant structures form and, for the highest concentration clustered structures, Kapitza resistance is observed to increase by more than a factor of 50. Our talk will conclude with an outline discussion of our efforts to incorporate atomics scale results into a microstructure informed continuum thermal transport model capable of capturing the effects of varying grain size distribution and varying Kapitza resistance on cumulative thermal conductivity. 1. J.-P. Crocombette, G. Dumazer, N. Q. Hoang, F. Gao, and W. J. Weber, Journal of applied physics 101, 023527 (2007).

13th U.S. National Congress on Computational Mechanics
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Title: Wall Stress Computations in Abdominal Aortic Aneurysms: A Clinically Feasible Approach

Author(s): Sevan Goenezen, *Texas A&M U.*; Jaime Zelaya, Amir Azarbal, Sandra Rugonyi, *OHSU*.

The risk of an abdominal aortic aneurysm (AAA) rupture is currently assessed based on a threshold diameter criteria. More precisely, if a maximum diameter of about 5 cm is exceeded, the patient is believed to be in danger and a surgical intervention follows. However, many aneurysms grow beyond 5 cm without rupturing, while others rupture before reaching this threshold diameter. Clearly, this is not a good criteria to assess aneurysm stability. From a mechanical point of view, wall stresses lead to material failure and should be utilized to assess the risk of an AAA rupture. Computation of AAA wall stresses is very complex as it requires the knowledge of the undeformed AAA geometry, boundary conditions (e.g. pressure and deformations), and the constitutive material model for the AAA tissue. In this presentation, we will demonstrate that we can determine the wall stress distribution of AAAs with a linear material model and small strain theory with higher accuracy [1] than utilizing conventional methods (e.g. nonlinear hyperelastic material models). The proposed procedure makes it feasible to utilize wall stress computations in a clinical environment due to its simplicity and efficiency. [1] J.E. Zelaya, S. Goenezen, A.F. Azarbal, and S. Rugonyi,“Improving the efficiency of abdominal aortic aneurysm wall stress computations,” PLOS ONE 9 7, 2014.

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Title: Phase-Field Modeling in Computational Bioengineering: Application to Tumor Angiogenesis and Cellular Migration

Author(s): Hector Gomez, Adrian Moure, Guillermo Vilanova, *U. Coruña*.

In this talk, I will try to illustrate the potential of phase-field modeling to solve problems in computational bioengineering. Phase-field modeling refers to a particular mathematical description of a system with evolving interfaces. The key idea is to introduce a new field, the so-called phase field, which is defined on the entire domain, locates the different phases and encodes the interfacial physics at once. The phase-field is approximately flat on the bulk phases and changes rapidly, where different phases meet, giving rise to the concept of diffuse-interfaces. The phase-field equations are inherently nonlinear with higher-order spatial derivatives that account for the interfacial forces. However, these equations are posed on a fixed domain, which greatly simplifies numerical discretization. I will show how the phase-field concept opens the door to efficient modeling of diverse biological phenomena, including cellular migration and tumor angiogenesis. In cellular migration, the phase field concept permits straightforward tracking of the cell's movement, and simple incorporation of the relevant forces, namely, surface tension, bending, myosin contraction, cell-substrate adhesion and filament protrusion. In tumor angiogenesis, the use of phase fields permits capturing the complicated three-dimensional patterns exhibited by capillaries triggered by malignant tumors. I will conclude my presentation by discussing other potential applications.

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Title: Multi-Scale Modeling and Simulation of Powder Compaction

Author(s): Marcial Gonzalez, *Purdue U.*.

Powder compaction plays a relevant role in many pharmaceutical, food, ceramic and metallurgical manufacturing processes, so much so that microstructure evolution during consolidation has direct impact on the end-product properties and performance. This process involves a variety of coupled physical mechanisms at the particle-scale (e.g., elasto-plastic deformations, adhesion, bonding, friction, and fracture) that govern the properties and performance of the final product (e.g., tablet hardness, swelling and disintegration for pharmaceutical powders pressed into solid tablets for oral administration). Therefore, it is of paramount importance to fundamentally understand these coupled mechanisms in order to optimize manufacturing processes and to improve product design. Predictive multi-scale modeling and simulation of microstructure formation and evolution during compaction of granular solids requires research efforts in three main fronts. First, the development of predictive constitutive models of inter-particle interactions that account for high levels of confinement and a variety of physical mechanisms. Second, the development of concurrent multi-scale strategies that combine a detailed description of the granular scale with the computational efficiency typical of continuum-level models. Third, the experimental characterization of particle's mechano-chemical properties required in the model. In this talk, I will present progress in these three fronts, including: (i) nonlocal contact formulations that overcome the typical, but unrealistic, assumption that contacts are independent regardless the confinement of the granular system [1], (ii) a particle mechanics approach which concurrently solves for contact forces at the granular scale, for nonlocal deformations at the mesoscale, and for static equilibrium at the macroscale [2], (iii) characterization techniques that utilize modeling and experimental methodologies in lockstep coordination with each other at the particle scale [3]. [1] Gonzalez M. and Cuitiño, A.M., "A nonlocal contact formulation for confined granular systems", Journal of the Mechanics and Physics of Solids, 60, 333–350, 2012. [2] Gonzalez M. and Cuitiño A.M., "Microstructure evolution of compressible granular systems under large deformations", under review, 2015. [3] Yohannes B., Gonzalez M., et al., "The role of fine particles on compaction and tensile strength of pharmaceutical powders", Powder Technology, 274, 372–378, 2015.

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Title: High-DImensional Bayesian Inference with Tensors

Author(s): Alex Gorodetsky, Youssef Marzouk, *MIT*.

Bayesian inference is an important component of uncertainty quantification, and state of the art methods for high dimensional Bayesian inference typically rely on sampling. Examples of such algorithms include Monte Carlo sampling, importance sampling, and Markov chain Monte Carlo. Samples obtained from these algorithms are then used for evaluating integrals of functions with respect to the posterior distribution. As an alternative to sampling algorithms, we propose to re-examine the utility of tensor product quadrature for Bayesian inference. Tensor product quadrature has several advantages over sampling, and these advantages include well defined error and convergence properties. Traditionally, the utility of tensor product quadrature in high dimensions suffers from the curse of dimensionality, where the number of quadrature nodes grows exponentially with dimension. In this work, we take advantage of recent techniques focusing on tensor decompositions to decrease the computational expense of quadrature in Bayesian computation from exponential growth to linear or polynomial growth with dimensions. The reduction in computational expense results from taking advantage of low rank structure based on the concept of separation of variables in various aspects of the Bayesian problem. We show the applicability of taking advantage of low rank structure in both dynamic data assimilation problems as well as in static inference problems. In the dynamic data assimilation, or filtering, context we show how the low rank nature of prediction and observation operators can lead to development of more accurate Gaussian filters for a small increase in computational expense. In the static Bayesian inference problem we take advantage of low rank structure of the posterior distribution itself, and demonstrate algorithm performance on a distributed, or spatial, parameter inference problem for an elliptic PDE often encountered when dealing with subsurface flows.

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Title: Accurate Estimation of Probability of Failure in Large-Scale Stochastic Structural Simulations

Author(s): Sonjoy Das, Kundan Goswami, *U. Buffalo*; Biswa N. Datta, *Northern Illinois U.*.

Estimating probability associated with extreme events typically requires millions or billions of samples. While importance sampling (IS) and similar methods can substantially reduce the number of samples, there is still a serious computational bottleneck particularly for large-scale structural simulations where a limited computational budget is typically available allowing one to run only a given number of forward simulations. In this work, we propose a modified IS scheme to accurately estimate the probability of failure given a certain computational budget. Another challenging task in the context of computing probability of failure is identification of the unknown failure domain in the input-variables space. In this work, we also present a scheme based on hierarchical clustering technique to identify this unknown failure domain. The proposed work is illustrated on active structural vibration controlled structural systems that require the concept of quadratic partial eigenvalue assignment problem. The proposed scheme is likely to guarantee the desired resilience level of the designed dynamic systems.

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Title: Thermomechanical and Electromechanical Analysis of Dislocations and Plasticity

Author(s): Robert Gracie, Oxana Skiba, *U. Waterloo*.

In this presentation, the first Dislocation Dynamics (DD) model capable of capturing the thermomechanical and electromechanical behaviour of a set of discrete dislocation will be presented. In DD models, the nucleation, motion, and interaction of a system of dislocations is explicitly simulated. Here, the eXtended Finite Element Method (XFEM) is leverage to create the first multiphysics DD simulations [1-3]. These microscale DD simulations provide insight into the observed macroscale plastic behaviour of metals and piezoelectric materials. For metals, XFEM is used as the basis for thermomechanical DD simulations, which provide insights into the underlying mechanisms of shear band temperature rises during high strain rate localization processes. For piezoelectric materials, XFEM is used as the basis for electromechanical DD simulations and explains how the direction of an applied electric field impacts hardening. In this presentation the numerical methods underpinned the XFEM multiphysics DD simulations will be presented and the effectiveness of this modelling strategy will be demonstrated. Lastly, the XFEM-DD simulations will be used to demonstrate/explain interesting macroscale plasticity phenomena in metals and piezoelectric materials. [1] Skiba, O, Gracie, R., and Potapenko, S. Electromechanical simulations of dislocations. Modelling and Simulation in Material Science and Engineering. Vol. 21, pp. 035003, 2013. [2] Gracie, R., Ventura, G., and Belytschko, T. A new fast method for dislocations based on interior discontinuities. International Journal for Numerical Methods in Engineering, Vol 69, pp. 423-441, 2007. [3] Gracie, R. and Belytschko, T. Concurrently Coupled Atomistic and XFEM Models for Dislocations and Cracks. International Journal for Numerical Methods in Engineering, Vol. 78, pp. 354-378, 2009.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Measure-Theoretic Parameter Estimation for Hydrodynamic Models

Author(s): Lindley Graham, Clint Dawson, *UT Austin*; Troy Butler, *U. Colorado-Denver*.

Since Hurricane Katrina (2005) there has been a marked increase in the quantity of field observations gather during and after hurricanes. There has also been an increased effort to improve our ability to model hurricanes and other coastal ocean phenomena. The majority of death and destruction due to a hurricane is from storm surge. The primary controlling factor in storm surge is the balance between the surface stress due to the wind and bottom stress. Manning's formula can be used to model the bottom stress with the Manning's n coefficient, a spatially dependent field. It would be impractical to estimate Manning's n over such a large physical domain. Instead given a computational storm surge model and a set of model observations one may seek to solve the inverse problem to determine an appropriate Manning's n field to use for predictive simulations. We leverage existing land cover classification data generated from high-resolution aerial photography to determine the spatial distribution of land cover classification which we consider certain. This forms our mesoscale representation of the Manning's n field. We seek to estimate the Manning's n coefficients for this parameterized field. We solve this inverse problem using a measure-theoretic approach applied to the ADCIRC storm surge model. We model uncertainty in the data as a probability measure on the data space. The corresponding model of uncertainty in the parameters is then a probability measure on the parameter space. Our goal is to solve the resulting stochastic inverse problem. In this application the dimension of the data space is smaller than the dimension of the parameter space. Thus, the inverse problem has set-valued solutions which we refer to as generalized contours. We can decompose the parameter space into directions along these generalized contours and directions transverse to the generalized contours. These correspond to unobservable directions and observable directions. We can similarly decompose the probability measure on the parameter space. The conditional probability density along the generalized contours cannot be uniquely determined from the model. Instead, we must assume an ansatz to determine the conditional probability density. We discuss the impact of the ansatz and the role of Bayesian analysis within this measure-theoretic approach.

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Title: Modelling Wave Propagation in Large Structures Using the Scaled-Boundary, Finite-Element Method

Author(s): Hauke Gravenkamp, *Fed'l. Inst. Materials Rsch. & Testing*.

This contribution discusses the concept of the Scaled Boundary Finite Element Method (SBFEM) in the context of the simulation of wave propagation phenomena. The SBFEM is a semi-analytical method requiring the discretization of the boundary of the computational domain only. It can be applied to both bounded and unbounded domains and offers a convenient and accurate way to model stress singularities. Particulary for large homogeneous structures, applying the SBFEM can reduce computational costs by orders of magnitude compared to standard Finite Element Analysis. We present recent developments and applications and discuss benefits and limitations of this method. Examples include the modelling of elastic waveguides, soil layers and applications in ultrasonic testing of materials.

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Title: The Parallel Wavelet Adaptive Multi-Resolution Representation (pWAMR) Method

Author(s): T. Grenga, S. Paolucci, *U. Notre Dame*.

The parallel Wavelet Adaptive Multiresolution Representation (pWAMR) method deals with the solution of PDEs that model particularly challenging multi-dimensional continuum physics problems having strong multi-scale character. The method provides a robust means of controlling spatial grid adaptation. Since the amplitudes of the wavelet representation provide a direct measure of the local error at each collocation point associated with a wavelet, the method is able to efficiently capture to any desired accuracy a wide range of spatial scales using a relatively small number of degrees of freedom by evolving the dynamically adaptive grid. Subsequently, high resolution computations are performed only in the regions where near-singularities or sharp transitions occur. In an effective fashion, the multilevel structure of the algorithm provides a simple way to adapt computational refinements to local demands of the solution, thus automatically producing verified solutions. The pWAMR algorithm is parallelized using a MPI-based domain decomposition approach suited to a wide range of distributed-memory parallel architectures. Most recent updates on the algorithm, and in particular on the evaluation of derivatives of the wavelet basis, enables good parallel performance. The use of the dynamically adaptive grid in conjunction with the parallel implementation provides the possibility of solving challenging multiscale physics problems. The method is applied to the solution of unsteady, compressible, reactive flow problems and includes multicomponent diffusive transport and detailed chemical kinetics models. Accuracy and performance of the method are examined on several test problems.

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Title: Fluid-Structure Interaction Models of Natural and Prosthetic Heart Valves

Author(s): Boyce E. Griffith, Amneet P. S. Bhalla, *U. North Carolina-Chapel Hill*.

It is well appreciated that many of the difficulties of prosthetic heart valves are related to the fluid dynamics of the replacement valve. For instance, unphysiological flow patterns generated by mechanical valve prostheses induce platelet activation and thereby necessitate the use of sustained anticoagulation therapy in patients who receive such devices. Fluid shear stresses also are involved in the deterioration of the materials used in bioprosthetic valves, which contributes to the relatively limited durable lifetime of such devices. Bioprosthetic valve leaflets also fail as the result of mechanical effects, including flexural stresses resulting from the large deformations of the valve leaflets during the cardiac cycle, and tensile stresses resulting from the substantial pressure loads imposed on the closed valve. Computational models of cardiac valve dynamics can predict the flow patterns of native, mechanical, and bioprosthetic valves, and also can predict the kinematics and loads experienced by the valve leaflets. Such models promise to improve our understanding of the dynamics of native and prosthetic valves by providing detailed information about flows and leaflet deformations and stresses that is not readily available from experimental or clinical imaging approaches. This talk will describe ongoing work to develop detailed fluid-structure interaction (FSI) models of heart valves, focusing on models of the native aortic valve as well as aortic valve prostheses. This work employs the immersed boundary (IB) method, which is a mathematical and numerical approach to modeling FSI. The IB method employs an Eulerian description of the momentum, viscosity, and incompressibility of the fluid-solid system along with a Lagrangian description of the deformations and stresses of the immersed structure. Although the conventional IB method describes elastic structures that are represented in terms of systems of elastic fibers that are typically discretized using nonlinear springs or beams, the IB method is not limited to such material descriptions. Extensions of the IB method have been introduced to treat structural models with experimentally constrained hyperelastic constitutive laws, and to treat immersed rigid structures. These extensions, along with improvements in discretization methods and solvers, are enabling increasingly realistic simulations of heart valve dynamics. Progress towards the development of experimentally validated IB models of the aortic valve will also be presented.

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Title: Multi-Scale Computational Modeling of Keratoconus Progression

Author(s): Rafael Grytz, *U. Alabama, Birmingham*; Sally Hayes, Craig Boote, Keith Meek, *Cardiff U.*.

Keratoconus is an ocular disease of unknown cause, which affects approximately 1 in 2000 people. At the macro-scale, the cornea thins, deforms into conical shape, and has a reduced stiffness. At the micro-scale, the anisotropic collagen architecture becomes disorganized due to a potential redistribution of collagen fibrils within the cornea. Increased levels of MMP9, inadequate cross-linking, and a reduction of the collagen fibril diameter have been reported in keratoconus. As the exact remodeling mechanisms are still unknown, we propose a multi-scale computational model to explore potential remodeling mechanisms that may underly keratoconus progression. We hypothesize that keratoconus is due to a weakening of the corneal collagen structure, which involves two mechanisms: (i) collagen fibril sliding and (ii) degradation. At the micro-scale, we propose strain-based rules for collagen fibril sliding and degradation with abnormal threshold values representing collagen weakening in keratoconus. At the macro-scale, we assume a multiplicative split of the deformation gradient into three parts: an elastic part, an isochoric remodeling part, and a growth part. The proposed growth and remodeling model is applied to a generic computational model of a normal human eye, which incorporates the anisotropic collagen architecture from X-ray diffraction measurements [1]. The model results show that, once initiated, collagen sliding leads to a progressive conical shaped protrusion as observed in clinic. Collagen fibril degradation increased at the cone causing a disorganization of the anisotropic collagen architecture as seen in X-ray diffraction experiments [1]. The predominant directions of collagen fibril sliding and degradation were perpendicular to each other at the apex. Corneal thinning occurred around the apex of the cone and was primarily caused by the sliding mechanism. The predicted region of corneal thinning was less extensive but matched the magnitude seen in clinic. The good agreement of the numerical results with clinical and experimental observations supports the notion that keratoconus progression is due to collagen fibril sliding and degradation. This is the first study to demonstrate that biomechanically-driven remodeling mechanisms can lead to the micro- and macro-structural changes observed in keratoconus. Reference [1] Hayes et al. 2007. A study of corneal thickness, shape and collagen organisation in keratoconus using videokeratography and X-ray scattering techniques. Exp. Eye Res. 84, 423-434.

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Title: Large-Scale Simulation for Self-Assembly of Crystalline Nanostructures with High Performance Computing

Author(s): Zhen Guan, John Lowengrub, *UC Irvine*; Sudhakar Pamidighantam, *Indiana U.; NCSA, U. Illinois* ; Hadrian Djohari, *Case Western Reserve U.*.

Reproducing synthesizing and assembling arrays of nanostructures with controlled morphologies and compositions is very important in the study of nanostructured materials, which are basis of many breakthrough technologies. Computational modeling is essential for understanding the complex fundamental processes underlying nanostructure growth and self-assembly. We exploits recent developments in phase field crystal (PFC) models and develops PFC-based models and computational methodology for modeling solid-vapor, liquid-vapor and faceted solid-liquid interfaces, which are commonly present during the growth of crystalline nanostructures. It needs to be pointed out that although PFC-based models allow larger domains to be simulated comparing with the traditional approach, the scale for the degree of freedom we are interested is still of trillion order and higher. Also governing equations derived from these models are complicated systems involving gradient, nonlinearity and convolution. These characters of the model pose challenges to current state-of-the-art computational methods in both numerical algorithms and high performance computing implications. We developed an unconditional stable scheme with almost optimal efficiency. We also implement it in an efficient parallel geometric multigrid solver. As the result the time consumption of the simulation is reduced significantly.

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Title: Modeling of Wave-Induced Slump Using Reproducing Kernel Particle Method

Author(s): Onlei Annie Kwok, *Nat'l. Taiwan U.*; Pai-Chen Guan, Chien-Ting Sun, Jia-Hong Jiang, Wen-Huai Tsou, *Nat'l. Taiwan Ocean U.*.

Natural earth slope and earth retaining structure near the coastal area may be subjected to slamming loads imposed by tidal waves. Surficial slope instability may be resulted if large impulsive slamming loads impact on the slope surface. On the other hand, deep-seated submarine slump can also be resulted if the tidal wave action continues for a prolonged period of time. These slumps can cause large displacements of water which can, in turn, generate tsunami waves. The modeling of wave-slope interaction requires the numerical method to be able to properly describe the free surface wave propagation, the nonlinear and fracture behavior of solid, and the fluid-structure interaction (FSI) of constantly evolving interface. Therefore, we propose using the consistent discretization of both fluid and solid by the reproducing kernel particle method (RKPM). The slope failure mechanism is described by the recently developed “semi-Lagrangian reproducing kernel particle method” (SLRKPM) [1]. The free-surface wave modeling is handled by the newly developed Smoothed RK hydrodynamics framework. Both developed codes have been tested to evaluate the reliability, and good agreement is observed by comparing the analytical, experimental and empirical solutions. The FSI is treated by a new contact scheme, which includes the gradient fluid-surface-identification algorithm, as well as the boundary-layer-solution-enriched surface force calculation method. Several benchmark problems are presented in this study to demonstrate the performance of the proposed method. The wave-induced gravity slump can be observed in the simulation results. The failure mechanism involves the general shear-band-type failure which emanates from the toe of the slope. Moreover, surficial slope damages can also be observed. 1. On-Lei Annie Kwok, Pai-Chen Guan, Wei-Po Cheng, Chien-Ting Sun, “Semi-Lagrangian Reproducing Kernel Particle Method for Slope Stability Analysis and Post-Failure Simulation,” KSCE Journal of Civil Engineering, January 2015, Volume 19, Issue 1, pp 107-115 Keywords: reproducing kernel particle method, free surface flow, hydrodynamic, slope stability, fluid-structure interaction

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Title: The Interplay Between Integration and Interpolation Errors in Finite Element Simulation of Wave Propagation

Author(s): Murthy Guddati, Ali Vaziri Astaneh, *NC State U.*; Vladimir Druskin, *Schlumberger Doll Rsch.*.

While the idea of reduced integration has long been used to counter the stiffening effect of finite element approximations, the past decade has seen renewed effort in this direction, specifically in the context of wave propagation problems. Modified integration has been used to reduce the dispersion error not only for linear elements [1,2], but also for higher order discretizations [3]. Similarly, midpoint point integration combined with linear interpolation is shown to preserve impedance leading to effective implementation of perfectly matched layers to simulate unbounded domains [4]. In this talk, we claim that the power of modified integration rules stretches beyond the two approaches described above. First, we show that the midpoint integrated linear finite element mesh, when bent into the complex space in a specific way, results in exponentially converging solution on the edges, leading to significant reduction in the computational cost [5]. Secondly, we show that the idea extends to higher order elements, leading to increased flexibility and broader applicability. The talk will contain the details of the proposed methods, the underlying mathematical rationale, as well as numerical examples illustrating the effectiveness of the methods. [1] M.N. Guddati and B. Yue (2004), "Modified integration rules for reducing dispersion in finite element methods," Computer Methods in Applied Mechanics and Engineering, 193, pp. 275-287. [2] A.V. Idesman, M. Schmidt, and J.R. Foley (2011), “Accurate finite element modeling of linear elastodynamics problems with the reduced dispersion error,” Computational Mechanics, 47, pp.555-572. [3] M. Ainsworth and H.A. Wajid (2010), “Optimally blended spectral-finite element scheme for wave propagation and nonstandard reduced integration,” SIAM Journal on Numerical Analysis, 48(1), pp. 346-371. [4] M.N. Guddati and K.W. Lim (2006), "Continued fraction absorbing boundary conditions for convex polygonal domains," International Journal for Numerical Methods in Engineering, 66, pp.949-977. [5] M.N. Guddati, V. Druskin, A. Vaziri Astaneh (2014), "Exponential Convergence through Linear Finite Element Discretization of Stratified Subdomains," Journal of Computational Physics (submitted).

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Title: Uncertainty Quantification in the Numerical Simulation of Particle-Laden Flows: The Impact of Using Phenomenological Viscosity

Author(s): Gabriel Guerra, Fernando Rochinha, Felipe Horta, Marta Mattoso, Renato N. Elias, Alvaro L. G. A. Coutinho, *U. Federal Rio de Janeiro*; Henrique F. da Costa, *U. Federal Rio de Janeiro*.

Particle-laden flows are a very complex natural phenomenon and considered one of the most responsible for sediment transport and deposition that lead to the formation of basins hosting oil reservoirs. Those turbulent flows are triggered by small differences in the fluid density induced by the presence of sediment particles. A detailed modelling of this phenomenon may offer new insights to help geologists to understand the deposition mechanisms and the final stratigraphic form of the reservoirs. The increasing reliance on numerical simulation for the analysis of these complex physical systems has led in recent years to a strong development of knowledge in this area. In this sense, Uncertainty Quantification (UQ) provides a framework to enable robust computer simulations that take into account the unavoidable uncertainties present in input parameters and in the model structure (model discrepancy). The present work extends the efforts of the authors to build a reliable computational model for the prediction of deposition of sediments transported by particle laden-flows. It presents a UQ analysis, employing a probabilistic perspective, to consider the impact of using phenomenological viscosity models on quantities of interest such as bottom shear stresses and deposition maps. Those models combine experimental observations with physical intuition and try to capture the influence of the sediment concentration on the local flow viscosity. Both parameter uncertainties and different forms of model discrepancy (stochastic spatial fields) are considered in the simulations through non-intrusive stochastic collocation methods while a parallel Navier-Stokes solver handles the underlying deterministic model. A scientific workflow management engine tool designed for high-performance computers supports the whole procedure.

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Title: Stochastic Continuum Modeling of Random Interphases Based on Atomistic Simulations: Application to a Nanoreinforced Polymer

Author(s): Thinh Le, Johann Guilleminot, Christian Soize, *U. Paris*.

In this work, we address the multiscale analysis of nanoreinforced polymers. For most of these materials, both experimental and numerical investigations have demonstrated the existence of a perturbed area, commonly called an interphase region, at the boundary between the filler and the matrix phase (see e.g. [1] [2]). This presentation specifically focus on the construction and identification of a stochastic continuum model for the interphase properties making use of an atomistic representation of the composite system. To this aim, a set of molecular dynamics (MD) simulations on a polyethylene-like polymer containing stiff nano-inhomogeneities is first performed. These simulations are used to determine the conformational properties of the polymer chains near the fillers, hence allowing for the construction of a suitable random field model [3]. The latter is subsequently identified by solving a statistical inverse problem involving the MD results. Finally, the impact of such random properties on the macroscale behavior is investigated through a stochastic homogenization procedure. References: [1] J. Berriot, F. Lequeux, L. Monnerie, H. Montes, D. Long and P. Sotta. Filler-elastomer interaction in model filled rubbers, a 1H NMR study. Journal of Non-Crystalline Solids, Vol. 307, 719-724, 2002. [2] D. Brown, V. Marcadon, P. Mélé and N.D. Albérola. Effect of filler particle size on the properties of model nanocomposites. Macromolecules, Vol. 41 (4), 1499-1511, 2008. [3] J. Guilleminot and C. Soize. Stochastic Model and Generator for Random Fields with Symmetry Properties: Application to the Mesoscopic Modeling of Elastic Random Media. SIAM Multiscale Modeling & Simulation, Vol. 11 (3), 840-870, 2013.

13th U.S. National Congress on Computational Mechanics
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Title: Reduced Basis Methods for Non-Local Diffusion Problems with Random Input Data

Author(s): Max Gunzburger, *Florida State U.*.

Nonlocal models have arise in a large number of applications such as the peridynamics model for solid mechanics, anomalous diffusion in subsurface flows, image processing, and machine learning. We consider a nonlocal model for diffusion having random input data. We reduced basis method for spatial approximation coupled to sparse grid stochastic collocation methods for stochastic approximation. Two reduced basis methods are determined using a greedy algorithm. The well posedness of the problem and convergence results for numerical approximations are proved and the efficiency of the methods developed are studied. Particular attention is paid to the effects of nonlocality on the complexity of the discretized systems. Numerical experiments are used to illustrate the theoretical results. Joint work with Qingguang Guan, Kuo Liu, Clayton Webster, and Guannan Zhang.

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Title: Doing Topology Optimization Explicitly and Geometrically: A New Moving Morphable Components Based Framework

Author(s): Xu Guo, Weisheng Zhang, Wenliang Zhong, *Dalian U. Tech.*.

In the present work, we intend to demonstrate how to do topology optimization in an explicit and geometrical way. To this end, a new computational framework for structural topology optimization based on the concept of moving morphable components is proposed. Unlike in the traditional solution frameworks, where topology optimization is achieved by eliminating unnecessary materials from the design domain or evolving the structural boundaries, optimal structural topology is obtained by optimizing the layout of morphable structural components in the proposed approach. One of the advantages of the proposed approach, which may have great potential in engineering applications, is that it can integrate the size, shape, and topology optimization in CAD modeling systems seamlessly. The approach can combine both the advantages of explicit and implicit geometry descriptions for topology optimization. It also has the great potential to reduce the computational burden associated with topology optimization substantially. Some representative examples are presented to illustrate the effectiveness of the proposed approach. 1. M. P. Bendsoe, N. Kikuchi, Generating optimal topologies in structural design using a homogenization method, Computer Methods in Applied Mechanics and Engineering, 71: 197-224, 1988. 2. M. P. Bendsoe, Optimal shape design as a material distribution problem, Structural Optimization, 1: 193-202, 1989. 3. M. Zhou, G. I. N. Rozvany, The COC algorithm, part II: topological, geometry, and generalized shape optimization, Computer Methods in Applied Mechanics and Engineering, 89: 309-336, 1991. 4. M.Y. Wang, X.M. Wang, D.M. Guo, A level set method for structural topology optimization, Computer Methods in Applied Mechanics and Engineering, 192: 227-246, 2003. 5. G. Allaire, F. Jouve, A.M. Toader, Structural optimization using sensitivity analysis and a level set method, Journal of Computational Physics, 194: 363-393, 2004. 6. X. Guo, W. S. Zhang, W. L. Zhong, Doing topology optimization explicitly and geometrically-a new moving morphable components based framework, Journal of Applied Mechanics, 81: 081009-1-081009-12,2014.

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Title: A Finite Element Model of Self-Sensing Piezoelectric Sensor for Damage Detection Undergoing Dynamic Finite Deformation

Author(s): Shu Guo, Somnath Ghosh, *Johns Hopkins U.*.

Multi-functional structures such as loading-bearing antennas and active skins of aircraft, which contribute to both device functionality and structure integrity, have received intensive interests as components of unmanned airborne vehicles (UAVs) due to the compact design and functionality. To analyze the multi-physics phenomena that occur in the multi-functional structures, a model that can couple transient electromagnetics field and dynamic finite deformation is necessary. An in-house high performance code has been developed to carry out multi-physics simulation and leading to design. The present work focuses on the multi-physics problem of a health monitoring structure using piezoelectric material undergoing finite deformation to detect damage under dynamic cyclic loading. The piezoelectric is designed to serve as an actuator as well as a sensor. The output electric signal, which combines the effect of both external dynamic loads and the applied electric field, is examined to identify the damage of the structure. Continuous and discontinuous phenomenological damage model are implemented to represent the hysteresis effect from cyclic loading and the damage associated with maximum strain energy along the loading history, respectively. Since the structure is assumed to experience finite deformation, the coupled system is studied in the material form. Balance of energy, thermodynamics laws and governing equations are investigated and the constitutive law is derived in the reference configuration. To analyze the piezoelectric damage detector, the coupled dynamic finite deformation and electric field are solved iteratively in a staggered way. Simulation is validated with existing analytical solution and commercial software. Analyses are carried out to study the detector performance in different cases with mixed dynamic loading and applied electric field.

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Title: Coupled Fluid-Flow/Mechanical/Fracture Simulations of Non-Planar Hydraulic Fracture Propagation

Author(s): Piyush Gupta, Armando Duarte, *U. Illinois, Urbana-Champaign*.

In this study, a fully coupled fluid-flow/mechanical/fracture formulation and an adaptive Generalized Finite Element Method (GFEM) are developed for the simulation of non-planar three-dimensional propagation of hydraulic fractures for hydrocarbon rich shale formations. Numerical simulation of hydraulically driven fracture propagation is challenging even in its most basic form because it involves coupling of at least three processes [1]: a) mechanical (rock) deformation induced by the fluid pressure on the fracture surfaces; b) flow of the fracturing fluid in the fracture and c) propagation of fracture, which is dependent on the current stress state of the rock. Rock deformation is usually modeled using the theory of linear elasticity [1, 5], specially for low permeability shale gas formations. Fluid flow inside the fracture is modeled using lubrication theory [1, 5]. Other factors, such as different magnitude of the in-situ stress state of the rock also have a significant effect on the direction and magnitude of the hydraulic fracture growth during early stages of fracturing treatment. Orientation of the well bore can also result in direction changes of initial fractures. All these factors affecting hydraulic fracture propagation are studied in detail in this work. Numerical solutions based on the proposed formulation and adaptive generalized FEM discretization are compared with asymptotic analytical solutions for the KGD [3, 4] and penny-shaped [2] models in toughness and storage dominated propagation regimes. The proposed methodology is able to reproduce the analytical solution with accuracy and computational efficiency. Examples where the fracture propagation exhibits sharp turns and non-planar behavior are also presented to show the versatility and robustness of the method. Keywords: Hydraulic Fracturing; Generalized finite element method; Fracture Mechanics; Coupled Formulation; Stress Intensity Factors. References [1] J. Adachi, E. Siebrits, A. Peirce, and J. Desroches. Computer simulation of hydraulic fractures. International Journal of Rock Mechanics & Mining Sciences, 44:739–757, 2007. doi: 10.1016/j.ijrmms.2006.11.006. [2] J. Desroches, E. Detournay, B. Lenoach, P. Papanastasiou, J. R. A. Pearson, M. Thiercelin, and A. Cheng. The crack tip region in hydraulic fracturing. Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences, 447(1929):39–48, 1994. doi: 10.1098/rspa.1994.0127. [3] J. Geertsma and F. de Klerk. A rapid method of predicting width and extent of hydraulically induced fractures. Journal of Petroleum Technology, 21:1571–1581, 1969. [4] S.A. Khristianovic and Y.P. Zheltov. Formation of vertical fractures by means of highly viscous liquid. In Proceedings of the Fourth World Petroleum Congress, pages 579–586, Rome, Italy, 1955. [5] A. Taleghani. Analysis of hydraulic fracture propagation in fractured reservoirs: An improved model for the interaction between induced and natural fractures. PhD Dissertation, University of Texas at Austin, 2009. Austin, TX, USA.

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Title: Numerical Simulations of Vehicular Impacts on Single- & Double-Faced W-Beam Guardrails on Sloped Median

Author(s): Matthew Gutowski, Ryan Baker, Daniil Kuvilla, Emre Palta, Howie Fang, *UNC Charlotte*.

Roadside and median barrier systems are an important part of roadside safety in that they reduce the total number of injuries and fatalities in highway crashes. Barrier systems achieve this by preventing errant vehicles from intruding into oncoming traffic or unsafe areas as well as safely redirecting the vehicles after an impacts. W-beam guardrails are the most commonly used semi-rigid barriers that allow the impact energy from a crash to be dissipated through the deflection and deformation of the guardrail. A common performance issue with the W-beam guardrails is snagging of the impacting vehicle, resulting in either a vehicle rollover or unsafe redirection. Since full-scale crash tests are costly and time consuming, it is not feasible to use them in the investigation of multiple crash scenarios. Recent advances in high performance computing and commercial simulation codes has made finite element (FE) modeling a viable option in roadside safety research. In this study, FE models of single-faced and double-faced W-beam guardrails [1] at different heights were evaluated under MASH Test Level 3 (TL-3) impact conditions. Two MASH TL-3 vehicle models, a small passenger car (1996 Dodge Neon) [2] and a large pickup truck (2006 Ford F-250) [3] were used to evaluate the vehicle's post-impact responses such as redirection, snagging, and spin-out. In addition, a double-faced guardrail with a lowered backside rail as well as the effects of a guardrail with horizontal curvature were evaluated. All guardrail configurations were evaluated at both the 29- and 31-inch heights using an impact speed of 62 mph (100 km/h) and a 25° angle. The guardrail deflection, vehicle response, and exit trajectories for all cases were assessed and compared. References: [1]Opiela, Ken; Kan, Steve; Marzougui, Dhafer (2007) "Technical Summary NCAC 2007-T-004 – Development of a Finite Element Model for W-beam Guardrails" National Crash Analysis Center. The George Washington University, Washington, D.C. [2]Opiela, Ken; Kan, Steve; Marzougui, Dhafer (2007) "Technical Summary NCAC 2007-T-007 – Development & Validation of a Finite Element Model for the 1996 Dodge Neon Passenger Sedan" National Crash Analysis Center. The George Washington University, Washington, D.C. [3]Mahadevaiah, Jadish (2008). "Finite element model development of Ford F-250 pick-up truck using laser-scanning Method, and its validation and application." Master's thesis. The George Washington University, Washington, D.C.

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Title: On Large-Scale Inverse Problems that Cannot Be Solved

Author(s): Eldad Haber, *U. British Columbia*.

In recent years data collection systems have improved and we are now able to collect large volume of data over vast regions in space. This lead to large scale inverse problems that involve with multiple scales and many data. To invert this data sets, we must rethink our numerical treatment of the problems starting from our discretization, to the optimization technique to be used and the efficient way we can parallelize these problems. In this talk we introduce a new multiscale asynchronous method for the treatment of such data and apply it to airborne Electromagnetics inverse problems.

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Title: Spacetime Discontinuous Galerkin Method for Hyperbolic Advection–Diffusion with a Non-Negativity Constraint

Author(s): Raj Pal, *Georgia Inst. Tech.*; Amit Madhukar, Robert Haber, *U. Illinois, Urbana-Champaign*; Reza Abedi, *U. Tennessee Space Inst.* .

Applications where the diffusive and advective time scales are of similar order give rise to advection–diffusion phenomena that are inconsistent with the predictions of parabolic Fickian diffusion models. Non-Fickian diffusion relations can capture these phenomena and remedy the paradox of infinite propagation speeds in Fickian models. In this work, we implement a modified, frame-invariant form of Cattaneo's hyperbolic diffusion relation within a spacetime discontinuous Galerkin advection–diffusion model. An h-adaptive spacetime meshing procedure supports an asynchronous, patch-by-patch solution method with linear computational complexity in the number of spacetime elements. This localized solver enables the selective application of optimization algorithms in only those patches that require inequality constraints to ensure a non-negative concentration solution. In contrast to some previous methods, we do not modify the numerical fluxes to enforce non-negative concentrations. Thus, the element-wise conservation properties that are intrinsic to discontinuous Galerkin models are defined with respect to physically meaningful Riemann fluxes on the element boundaries. We present numerical examples that demonstrate the effectiveness of the proposed model, and we explore the distinct features of hyperbolic advection–diffusion response in subcritical and supercritical flows.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Adaptive Immersed Nurbs Method for Fluid-Structure Interaction

Author(s): Elie Hachem, Youssef Mesri, *Mines Paristech* .

Immersed methods for Fluid Structure Interaction (FSI) are gaining popularity in many scientific and engineering applications. However, for problem involving complex geometries, the accuracy can be compromised and if mesh adaptation near the interface is applied, it remains difficult to obtain and consumes time and resources. We propose in this work a new adaptive immersed method based on the use of Non Uniform Rational B-Splines (NURBS). Indeed, the immersion of any complex object described usually by surface meshes is replaced by the direct use of the Computer Aided Design (CAD) definition keeping the quality of its analytical description. In practice, it eliminates the cost of the surface mesh generation step, increases the accuracy, reduces the complexity and enables setting easily a Fluid-Structure application. The interactions are then modelled by introducing an extra stress in the momentum equation. The obtained three-field velocity, pressure and stress system is solved using a new stabilized finite element method. Finally, we discuss the advantageous of this unified formulation and its ability to describe different kind of interactions and type of flows using several 2D and 3D benchmarks.

13th U.S. National Congress on Computational Mechanics
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Title: Uncertainty Quantification of Lithium-Ion Batteries

Author(s): Mohammad Hadigol, *U. Colardo, Boulder*; Alireza Doostan, Kurt Maute, *U. Colorado, Boulder*.

We introduce a fast uncertainty quantification (UQ) approach to study the effects of various sources of uncertainty on the performance of lithium-ion batteries (LIBs) described by an electrochemical model. Our proposed UQ approach, based on sparse polynomial chaos (PC) expansions, allows us to obtain converged solution statistics using a fairly small number of calls to the LIB model. It additionally enables us to identify the most important model parameters dominating the variation of quantities of interest, such as cell capacity, cell voltage, and concentrations, by performing a global sensitivity analysis. Such information is of particular interest for developing efficient battery materials and for designing cell assemblies. Moreover, our stochastic LIB model provides a general framework to study the propagation of input uncertainties through the cell as a function of the discharge process. This provides detailed information on the stochastic behavior of the cell over the entire duration of discharge. The performance of our proposed UQ approach for LIBs is explored via a numerical example. Specifically, we consider a LiC6/LiCoO2 cell with a total of 19 independent random inputs describing the uncertainty in porosity, solid particle size, Bruggeman coefficients?, lithium-ion transference number, salt diffusion coefficients in solid and liquid phases, electronic conductivity of the solid phase, reaction rate constants, and lengths of electrodes and separator. In this example, we show that our method only requires 1000 samples to obtain an accurate PC approximation of the cell capacity, voltage, and liquid and solid phase concentrations. We present our results for three different discharge rates of 0.25C, 1C, and 4C to study the effects of discharge rate on various quantities of interest. As we demonstrate through this example, discharge rate is a key factor in determining the most important random inputs.

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Title: Analysis of Flexoelectric Effect with Boundary Element Method

Author(s): Ali Hadjesfandiari, Arezoo Hajesfandiari, Gary Dargush, *SUNY Buffalo*.

It is well known that classical continuum mechanics cannot predict the behavior of materials for very small length scales. Therefore, we need to use consistent size-dependent continuum mechanics, which accounts for the length scale effect due to the microstructure of materials [1]. This enables us to develop consistent size-dependent theories in many multi-physics disciplines, such as flexoelectricity or piezoelectricity [2]. In this consistent theory, the electric field couples not only with strain, but also with mean curvature. Interestingly, we find that the electrical polarization can exist in centrosymmetric materials, such as isotropic dielectric materials [3]. Here we develop a two-dimensional boundary element formulation for flexoelectricity or size-dependent piezoelectricity in isotropic dielectric materials. This model is based on the new general reciprocal theorem for the equilibrium states of linear elastic size-dependent piezoelectric materials under different mechanical and electrical loadings [2]. The flexoelectricity effect is specified by two extra material properties: length scale and flexoelectric coefficient. In addition, we discuss the numerical implementation of the flexoelectricity boundary element method. Then, we apply this flexoelectric boundary element formulation to several computational examples to validate the numerical implementation and to explore flexoelectric couplings. References [1] A.R. Hadjesfandiari, G.F. Dargush, Couple stress theory for solids, International Journal of Solids and Structures, 48 (2011) 2496-2510. [2] A.R. Hadjesfandiari, Size-dependent piezoelectricity, International Journal of Solids and Structures, 50 (2013) 2781-2791. [3] Sh.M. Kogan, Piezoelectric effect during inhomogeneous deformation and acoustic scattering of carriers in crystals, Soviet Physics, Solid State, 5 (1964) 2069-2070.

13th U.S. National Congress on Computational Mechanics
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Title: Fourier Law with Embedded Discontinuity

Author(s): Ehsan Haghighat, S. Pietruszczak, *McMaster U.*.

Modeling of discontinuities is one of the most cumbersome tasks within the standard finite element framework, mainly due to the required remeshing-node duplicating for tracing the discontinuity interface. Over the last decade, the problems involving the presence of discontinuities have been often approached using the extended finite element method. This approach has been applied to a wide range of problems including coupled analyses such as heat/flow transfer, hydro-mechanical interaction, etc. Although the approach does not require any remeshing, dealing with additional enrichments functions poses some difficulties in terms of implementation. In this study, a Fourier law with embedded discontinuity is introduced for discrete modeling of discontinuities in flow/heat transfer problems. The new constitutive law is obtained by homogenizing the analytical representation of discontinuous flux around the crack and imposing the impermeability constraint. The procedure leads to a simple constitutive model that can be used for a mesh-independent modeling of discontinuities in heat transfer and/or fluid flow problems. A numerical example, which includes multiple randomly distributed impermeable layers, is provided to demonstrate the efficiency of the proposed methodology. The constitutive model can be defined by incorporating the notion of anisotropy. Thus, it can be used with any available anisotropic flow/heat representation without the need for dealing with additional degrees of freedom or remeshing.

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Title: Calculation of Stress Intensity Factor Using Meshfree Method with Dynamic Bubble System

Author(s): Seiya Hagihara, Yutaka Hayama, Shinya Taketomi, Yuichi Tadano, *Saga U.*.

The purpose of the present study is to calculate the stress intensity factors for crack problems using the element free Galerkin (EFG) method with nodal relocation method in which nodes adaptation is similar to molecular dynamics (dynamic bubble system). It is necessary to estimate error of numerical solutions of the EFG method for adaptive analyses to evaluate accuracy of it. Error estimation is performed according to Zienkiewicz-Zhu error estimator. Both adding nodes and relocating nodes by the dynamic bubble system are applied to the EFG method. When nodes are added near the stress concentrated region, they sometimes make the node density change from roughness to fineness extremely. This jumps of the nodal density lead results to lower accuracy. Nodes have to be controlled after adding nodes to improve higher accuracy solutions. The nodal relocation method is applied to smooth the distribution of nodes in domain and boundary of an analysis model. The dynamic bubble system for the FEM of which nodes are automatically relocated by the nodal relocation method is applied to the adaptive analysis and mesh generation. The physically interbubble forces in the nodal relocation method are determined by associating with the calculated posteriori error. The calculations of the EFG method can be repeated again after the posteriori error estimation. After repeating calculation, the solution is expected to become close to high precision solution. In this paper, the adaptive EFG method with the dynamic bubble system is applied to calculate the J-integral of crack problems which have the stress singularity at the vicinity of crack-tip. J-integrals are calculated in an each node allocation and on an each integral path.

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Title: A First-Order Conservation Law Formulation for Lagrangian Fast Solid Dynamics in OpenFOAM

Author(s): Jibran Haider, Antonio Javier Gil, Chun Hean Lee, Javier Bonet, *Swansea U.*.

Over the past few decades, computational fast solid dynamics has become an increasing share of interest in major engineering industries, namely aerospace, automotive, biomedical, defense and software industries. Traditionally, the displacement based formulation [1], typically discretised using Finite Element Method, has been employed to carry out the computational simulations for relevant applications. However, several drawbacks associated with the classical formulation need to be addressed: (1) Reduced order of convergence for derived variables; (2) High frequency noise in the vicinity of sharp spatial gradients; (3) Numerical instabilities associated with volumetric locking, shear locking and spurious hydrostatic pressure fluctuations. Within the OpenFOAM environment, it is essential to point out that the existing cell centred solid mechanics solver [1] is only capable of solving linear elastic infinitesimal deformations. Extension to large deformation framework using traditional formulation still remains unclear due to the shortcomings mentioned above. One of the main novelties in this paper is to develop a robust mixed solid solver, borrowed from the CFD community, for the numerical analysis of large strain fast solid dynamics. Following [2, 3], a mixed momentum/strains formulation written in a form of first order conservation laws will be employed. A successful implementation of this formulation in OpenFOAM, an open source cell centre based finite volume code in C++, has been carried out. The presence of jump in properties at the cell interfaces motivates the use of a Riemann solver by introducing an upwind bias into the evaluation of the numerical contact flux. A series of benchmark cases have been examined to illustrate the robustness of the proposed methodology. This formulation alleviates numerical instabilities associated with locking and pressure oscillations, and more importantly, yields equal order of convergence for velocity and stresses. References: [1] H. Jasak and H. G. Weller. Application of the finite volume method and unstructured meshes to linear elasticity. IJNME, 48, 267–287, 2000. [2] C. H. Lee, A. J. Gil and J. Bonet. Development of a cell centred upwind finite volume algorithm for a new conservation law formulation in structural dynamics. Computers and Structures, 118, 13–38, 2014. [3] M. Aguirre, A. J. Gil, J. Bonet and A. A. Carreno. A vertex centred finite volume Jameson-Schmidt-Turkel (JST) algorithm for a mixed conservation formulation in solid dynamics. JCP, 259, 672–699, 2014.

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Title: On the Numerical Treatment of Fine-Scale Interface Variables in Multi-Scale Interface Formulations

Author(s): Layla Amaireh, *Applied Science U.*; Ghadir Haikal, *Purdue U.*.

In a number of multi-scale Finite Element formulations for interface problems, fine-scale variables are higher-order functions, defined over the interface, that are introduced to increase the accuracy in capturing interface fields. The inclusion of higher-order interface variables, however, increases the numerical cost associated with the accurate representation of nonlinear interfacial effects such as frictional contact, particularly in the presence of material and geometric nonlinearities. In this presentation, we discuss an effective approach for the numerical treatment of multi-scale fields in interface problems such as frictional contact and the coupling of non-conforming meshes that balances the requirements of accuracy and algorithmic efficiency. We present our implementation in the context of the Enriched Discontinuous Galerkin Approach (EDGA), which was proposed in (Haikal and Hjelmstad, 2010) for contact problems and the coupling of non-conforming meshes. This method implements an element-level surface enrichment along with an interface stabilization procedure based on the Discontinuous Galerkin formulation to enable a two-pass approach for enforcing strong geometric compatibility conditions while ensuring weak continuity of surface tractions without introducing dual interface fields. We show that an efficient treatment of interface variables can improve algorithmic performance and circumvent numerical issues encountered in the presence of large deformations and nonlinear material behavior. References G. Haikal and K. D. Hjelmstad, “An enriched discontinuous Galerkin formulation for the coupling of non-conforming meshes,” Finite Elements in Analysis and Design, Vol. 46, No. 6, pp. 496-503, 2010.

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Title: Finite-Element Method for Timoshenko Beams Within Consistent Couple Stress Theory

Author(s): Arezoo Hajesfandiari, Ali Hadjesfandiari, Gary Dargush, *SUNY Buffalo*.

As the scale of structural systems is reduced to micro- or nano-levels, response tends to become size-dependent and new theory is required to extend the reach of continuum mechanics to such scales. This motivates the development of size-dependent continuum theory, such as the linear isotropic couple-stress theory we consider here [1], as the basis for studying multi-scale and multi-physics phenomena. In this couple-stress theory, there is a new material property with the dimensions of length. Inclusion of couple-stress effects only becomes critical for characteristic geometry on the order of that length. The new consistent couple stress theory has resolved many of the problems that previous size-dependent continuum theories have had [1]. Here we develop a variational principle for Timoshenko beam model based on the consistent couple-stress theory. This formulation provides a base for developing a couple-stress finite element approach for beam bending. We notice that this development combines the features of classical Euler–Bernoulli and Timoshenko beam theories, by retaining of both slope and shear angle as degrees of freedom along with the transverse deflection. We apply the formulation to a 2-node Timoshenko beam element and investigate the effect of couple stress in cantilever beam. Due to shear and curvature locking, we also investigate the alternative methods to improve the performance of the finite element method for beams when depth of the cross section becomes small. References [1] A.R. Hadjesfandiari, G.F. Dargush, Couple stress theory for solids, International Journal of Solids and Structures, 48 (2011) 2496-2510.

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Title: Hyperelastic Elastography in a Large-Scale Bayesian Inversion Setting

Author(s): Jack S. Hale, Stéphane P. A. Bordas, *U. Luxembourg*; Patrick E. Farrell, *Oxford U.*.

We consider the problem of recovering the material parameters of a hyperelastic material [1] in the Bayesian inversion setting. In the Bayesian setting we can extract the statistics associated with various sources of uncertainty, including noise, experimental deficiencies and incomplete observations of the domain. This will allow medical practitioners to make superior diagnostic decisions when presented with a quantitative measure of uncertainty in the recovered parameters. On the assumption of a Gaussian additive noise model, a Gaussian prior and a linear forward model, the posterior distribution of the material parameters given the observations will also be Gaussian. To ensure that the assumption of a linear forward model is valid, and that the posterior is approximated sufficiently well by a Gaussian distribution, we place a limit on the strain regime in which our current methodology applies. We are developing MCMC methods for exploring the non-Gaussian statistics of the posterior distribution. In the linear case, the covariance matrix of the posterior distribution is then characterised by the inverse of the Hessian of the objective functional evaluated at its minimiser. To extract statistical information from the large and dense Hessian we perform a low-rank approximation of the Hessian [2]. The eigenvectors associated with the lowest eigenvalues are the directions in parameter space that are least constrained by the observations. We implement this work within the dolfin-adjoint [3] software package. We derive the MPI-parallel finite element discretisation of the forward, adjoint (1st and 2nd order), and tangent linear models using the high-level differentiation tools available within the FEniCS project. We show results demonstrating the effects of partial observations and poor experimental design on the reliability of the recovered parameters. [1] N. H. Gokhale, P. E. Barbone, and A. A. Oberai, “Solution of the nonlinear elasticity imaging inverse problem: the compressible case,” Inverse Problems, 10.1088/0266-5611/24/4/045010 [2] H. P. Flath, L. C. Wilcox, V. Akçelik, J. Hill, B. van Bloemen Waanders, and O. Ghattas, “Fast Algorithms for Bayesian Uncertainty Quantification in Large-Scale Linear Inverse Problems Based on Low-Rank Partial Hessian Approximations,” SIAM J. Sci. Comput., 10.1137/090780717 [3] P. Farrell, D. Ham, S. Funke, and M. Rognes, “Automated Derivation of the Adjoint of High-Level Transient Finite Element Programs,” SIAM J. Sci. Comput., 10.1137/120873558

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Title: Developing Methods to Effectively Compare Atomistic Simulations of Dislocations and Dislocation Interactions

Author(s): Lucas Hale, Chandler Becker, *NIST*; Yuri Mishin, *George Mason U.*.

A framework of standardized methods is being developed in order to properly investigate dislocations and dislocation-point defect interactions using molecular dynamics. Classical molecular dynamics simulations are uniquely suited for studying dislocation interactions as the simulations provide the necessary atomic level description of the defects involved, along with the capability of observing dynamic behaviors at finite temperatures. However, the current methods used for such investigations are often not consistent or easily comparable and depend strongly on the underlying method and atomistic potential chosen. Our framework is designed to assist in the selection and development of classical interatomic potentials that best predict physically realistic dislocation plasticity behaviors. To support future endeavors into new materials of interest, the methods are being constructed in a generalized manner as opposed to focusing on a particular materials system. Additionally, by utilizing the framework for dislocation-point defect interaction studies, the usefulness and (current) limitations of atomistic studies of these interactions is explored. We will explain the system and demonstrate with initial studies involving metallic materials.

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Title: A Parallel Algorithm for Sparse Matrix Triple Product

Author(s): venkata arikatla, suvranu de, *RPI*; tansel halic, *UCA*.

Multigrid techniques play an integral part of many high performance codes. They are used in many areas for solving system of equations as they are known to possess good convergence properties. Most such algorithms involve Galerkin triple product of sparse matrices. In this paper we propose an algorithm to efficiently process such sparse triple products in parallel. The algorithm is based on generating a map that records the source and destination of non-zero block of entries while assuming that the underlying problem topology remains unchanged during the solution process. The proposed method eliminates the synchronization requirements of the previously proposed algorithm. Tests performed on the matrices generated from linear finite element elasticity matrices with varying mesh sizes showed better scalability in comparison to the previously proposed algorithm. The proposed algorithm shows promise to be extended to distributed memory systems as well as cases in which the underlying problem topology may undergo modification during solution.

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Title: Continous Fiber Thermoplastic Modeling and Simulation at Processing Temperatures

Author(s): Eduardo Guzman-Maldonado, Nahiene Hamila, Philippe Boisse, *INSA Lyon*.

CFRTP prepreg laminates thermoforming (Continuous Fiber Reinforcements and Thermoplastic Resin) is a fast composite manufacturing process. The development of a thermoforming process is complex and expensive to achieve by trial/error. In this work, a new visco-hyperelastic model for the simulation of thermoforming and stamping of CFRTP composites is presented. This model is formulated within the framework of non-linear continuum mechanics and is based on the generalization of the Maxwell linear viscous model applying the concept of internal variables. The strain energy density function is decomposed into three deformation modes using the definition of physical invariants. We show that viscoelastic behavior is mainly observed in in-plane shear deformation. In-plane shear characterization is performed using an improved Bias-Test set up at different temperatures. The identification of material parameters is carried out with the Levenberg-Marquardt algorithm for fitting experimental results. Finally, a thermoforming finite element simulation is presented in order to analyze the influence of temperature and the rate displacement of the process.

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Title: Large Eddy Simulations of Reactive Tracers in the Oceanic Mixed Layer

Author(s): Peter Hamlington, Katherine Smith, Nikki Lovenduski, *U. Colorado-Boulder*; Baylor Fox-Kemper, *Brown U.*.

Reactive tracers such as plankton and carbonate chemical species play important roles in the ocean carbon cycle. These tracers react primarily in the mixed layer, where air-sea gas exchange occurs and light is plentiful for photosynthesis. It is well known that there can be substantial heterogeneity, or “patchiness,” in the spatial distribution of ocean tracers, but the contribution of sub-kilometer scale turbulent processes to these distributions remains poorly understood. In this scale range, both submesoscale (100m - 10km), largely geostrophic, mixed layer eddies and small-scale, three-dimensional turbulence are active, resulting in substantial scale complexity from which tracer heterogeneity can arise. In this talk, we use results from two sets of numerical simulations in order to examine tracer characteristics and evolution in the presence of realistic mixed layer ocean turbulence. In the first set of simulations, we perform large eddy simulations (LES) of the spin-down of a large-scale temperature front on horizontal scales from 20km down to 5m. These simulations are used to understand the characteristics and evolution of tracers released at different depths in the mixed layer and tracers fluxing across the air-sea interface. The simulations include the effects of wave-driven Langmuir turbulence by solving the wave-averaged Boussinesq equations with an imposed Stokes drift velocity. In the second set of simulations, we perform LES of idealized biogeochemical tracers in the oceanic mixed layer from scales of hundreds of meters down to below one meter. By examining different tracer sources, flux rates, reaction mechanisms, and reaction time scales in these simulations, we connect the coupled turbulence-reaction dynamics with spatial, spectral, and statistical properties of the resulting tracer fields. Based on results from both sets of simulations, we highlight the dependence of tracer properties on mixed layer turbulent processes occurring at different scales, including vertical mixing by meter-scale Langmuir turbulence and kilometer-scale stirring by submesoscale eddies, fronts, and filaments. Eddy diffusivities are calculated for each of the tracers and the implications of the simulation results for parameterizations of submesoscale reactive tracer dynamics in large-scale climate simulations are discussed.

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Title: GPU-Based Parallel Algorithms for Simulation of Electro-Surgery Procedures in Real-Time

Author(s): Zhongqing Han, Venkata S. Arikatla, Suvranu De, *RPI*.

1. Introduction Physically accurate soft tissue cutting simulation is at the core of electro-surgery simulation in which the interplay of the electrical, mechanical and thermal properties of biological tissues needs to be captured. However, the changes of interfacial topology and tissue state cannot be easily tracked. The level set method which was originally introduced by Osher and Sethian has been proven to be efficient for tacking moving interfaces. The basic idea is to represent the dynamic interface implicitly and embed it as the zero level set of a time-dependent, higher dimensional function. The interface is evolved with the velocity field, which can be correlated with other physical parameters. A major limitation for a level set model is the expensive computational complexity, rendering it less feasible in a real-time interactive simulation. This can be overcome by the parallelizable characteristic of the level set procedures. 2. Methods In the level set framework, there are three major procedures: level set update, re-initialization and surface rendering. Re-initialization is used to maintain the level set function as signed distance, which is important and time consuming. Surface rendering of a high resolution level set is also computationally expensive. A localized, parallel level set method is proposed to speed up the cutting simulation. Our algorithm: (1) employs the electrical energy based velocity field to limit the active computational domain to the minimal set of changing elements; (2) uses GPU to parallelize the re-initialization procedure and (3) uses a high-speed CUDA based marching cubes to render the zero level set surface. 3. Results We have presented a GPU based level set algorithm for real-time electro-surgery simulation. Evolving with velocity field controlled by the input energy, the level set offers substantially greater physical fidelity of the cutting simulation and also provides different cutting shapes under different scenarios, which is required by different tissue effects in electro-surgery. References [1] S. Osher, J. Sethian, Level Set Methods and Dynamic Implicit Surfaces, Springer-Verlag, New York, NY, 2002. [2] M. Eyiyurekli, D. E. Breen, Data Structures for Interactive High Resolution Level-set Surface Editing, In Proceedings of the Conference on Graphics Interface, 95-102. [3] M. Roberts, J. Packer, M. C. Sousa etc. A Work-Efficient GPU Algorithm for Level Set Segmentation, Proc. Conf. High Performance Graphics, 123-132, 2010.

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Title: Phase-Field Fracture Modeling of Microsturcutres with Random Void Distribution

Author(s): Tong-Seok Han, Sang-Yeop Chung , *Yonsei U.*; Xiaoxuan Zhang , Christian Linder , *Stanford U.*.

The computational simulation of crack propagation often suffers difficulties due to singularities which destabilizes the numerical solution process. The complexity becomes more involved when multiple crack propagation is required to accurately describe a material behavior during degradation. When multiple crack initiation locations and propagation paths cannot be predefined such as in the case of microstructures with random voids, the computational modeling of crack propagation becomes even more challenging. In this work, a diffusive crack model, i.e., the phase field fracture model [1-3], is applied to multiple microcrack propagation simulation in cementitious materials with random void distribution. The correlation between the void distribution characteristics, crack patterns and strength prediction could be confirmed, and the potential of the phase field model for simulating multiple crack propagation problems for evaluating material properties is identified. References [1] G.A. Francfort, J.-J. Marigo, Revisiting brittle fracture as an energy minimization problem, Journal of the Mechanics and Physics of Solids 46 (1998) 1319-1342. [2] B. Bourdin, G.A. Francfort, J.-J. Marigo, Numerical experiments in revisited brittle fracture, Journal of the Mechanics and Physics of Solids 48 (2000) 797-826. [3] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Computer Methods in Applied Mechanics and Engineering 199 (2010) 2765-2278.

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Title: A Two-Dimensional Surface Model for Near-Wall Transport in the Large Arteries

Author(s): Kirk B. Hansen, Shawn C. Shadden, *UC Berkeley*.

Although coagulation is a complex process involving dozens of reactive species, the initiation phase of thrombin formation can be modeled as a rate-limited first-order kinetic reaction initiated at a thrombogenic surface on the vessel wall. Thrombogenic potential can therefore be approximated as the surface concentration of a single species released from the vessel wall at a constant rate. In large arteries, this transport is characterized by high Schmidt numbers (Sc ~ 1000) and therefore thin concentration boundary layers. Additionally, computational models of the full domain must resolve both advection-dominated high-Peclet regions and diffusion-dominated near-wall regions, posing numerical difficulties. As opposed to the flow problem, which is fully three-dimensional (3D), this transport problem is primarily two-dimensional (2D) and limited to a small near-wall region. In this work, we present a multiscale approach that reduces the 3D transport problem in large arteries to a 2D model on the surface manifold of the vessel wall. By assuming that transport is confined to a thin boundary layer near the vessel wall, and using an analysis similar to the von Karman integral method, the 3D transport equation is reduced a 2D surface transport equation. This equation is similar to the 3D version, except that velocity is replaced by wall shear stress, which is not divergence-free, and the advective term becomes non-linear. This method is used to model transport in abdominal aortic aneurysms, and the results are compared to those obtained by solving the full transport equations. Qualitatively, high values from the surface model seem to correlate well with those from the full simulation. This indicates that these regions may be especially susceptible to stasis-induced coagulation, although further investigation with a more comprehensive model is necessary. In its present form, this model can be used to help elucidate the relationship between wall shear stress and near-wall transport, as well as to investigate the influence of diseased vasculature on transport in the large arteries.

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Title: Progress on Manycore Multiphysics Simulation in Albany Using the Kokkos Portable Hardware Abstraction Library

Author(s): Andrew Bradley, Irina Demeshko, Glen Hansen, Alejandro Mota, Andy Salinger, Irina Tezaur, *Sandia Nat'l. Lab.*; Brian Granzow, *RPI*.

Albany is a multiphysics framework that supports a wide variety of application physics areas including heat transfer, fluid dynamics, structural mechanics, plasticity, quantum device modeling, climate modeling, and many others. The code, which employs advanced preconditioned nonlinear solution techniques and implicit methods, demonstrates strong scalability using MPI on problems exceeding a billion degrees of freedom run on current high performance computing systems. Recently, we have embarked on a process of reengineering the structure of Albany to provide high performance on multicore heterogeneous architecture computers that are becoming increasingly prevalent. Rather than optimize the code for a specific architecture, we have chosen to employ the Trilinos Kokkos hardware abstraction library, which provides a generic interface that hides machine specific details across various multicore and GPU coprocessor architectures. In this talk, we discuss various implementational details involved in integrating the Kokkos library into a modern implicit multiphysics code, and compare the code’s performance on different HPC platforms. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: An Assumed Strain-Based Moving Particle Finite Element and Extensions

Author(s): Su Hao, *ACII, INC.*.

The Moving Particle Finite Element Method (MPFEM) that combines a partition of unity with generalized finite element shape functions has been further developed using an assumed strain formulation derived based on a Hu-Washizu variation principle-based weak form solution, by which the arbitraries in meshless-based methodology, for examples, those in defining the dimension of interpolation window and selection of window function, are quantified through the minimization of an assistant potential under orthogonal condition. Extension to phase-field method and applications to engineering problems will be discussed. [1] S. Hao, W. Liu, T. Belytschko,“ An Assumed Strain Moving Particle Finite Element and Application to Fracture in Polycrystalline System”, manuscript submitted at 2010 and to be revised based on review comments. [2] Hao, S., W.K. Liu, and T. Belytschko, Moving particle finite element method with global smoothness. International Journal for Numerical Methods in Engineering, 2004. 59(7): p. 1007-1020. [3] Hao, S., Park, H. S., Liu, W. K., Moving particle finite element method. International Journal for Numerical Methods in Engineering, 2002. 53(8): p. 1937-1958. [4] Hao, S., Liu, W. K., Moving particle finite element method with superconvergence: nodal integration formulation and applications. Comput. Methods Appl. Mech. Engrg., 2006. 195: p. 6059-6072. [5] Simo, J.C. and T.J.R. Hughes, On the Variational Foundations of Assumed Strain Methods. Journal of Applied Mechanics-Transactions of the Asme, 1986. 53(1): p. 51-54. [6] Oden J. T. and Reddy J. N., Dual-complementary variational principles in mathematical physics, Int. J. Engr. Sci., 12(1), 1974, pp.1-29

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Title: Nitsche Methods for Plate Bending

Author(s): Isaac Harari, *Tel Aviv U.*.

An efficient procedure for embedding kinematic boundary conditions in plate bending is based on a stabilized variational formulation, obtained by Nitsche's approach for enforcing boundary constraints. Work-conjugate pairs weakly enforce kinematic boundary conditions. For thin plate problems, the absence of kinematic admissibility constraints allows the use of non-conforming meshes with non-interpolatory approximations, thereby providing added flexibility in addressing higher continuity requirements. The use of a scaling factor leads to a formulation with a single stabilization parameter. The enforcement of tangential derivatives of deflections obviates the need for pointwise enforcement of corner values in the presence of corners. The single stabilization parameter is determined from a local generalized eigenvalue problem, guaranteeing coercivity of the discrete bilinear form. The accuracy of the approach is verified by representative computations with bicubic B-splines, providing guidance to the determination of the scaling and exhibiting optimal rates of convergence and robust performance with respect to values of the stabilization parameter. For shear-deformable plates, the absence of kinematic admissibility constraints facilitates the use of approaches that are insensitive to shear locking. Again, the use of a scaling factor leads to a formulation with a single stabilization parameter, which is determined from a local generalized eigenvalue problem, guaranteeing coercivity of the discrete bilinear form.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Time-Dependent Viscoelastic Multiphase and Free Surface Flows with a Stabilized Finite-Element Method

Author(s): Daniel Hariprasad, Kristianto Tjiptowidjojo, *U. New Mexico*; Rekha Rao, P. Randall Schunk, *Sandia Nat'l. Lab.*; Peixi Zhu, Matthew Balhoff, *UT Austin*.

One standard approach for applying the finite element method to viscoelastic systems is the discrete elastic-viscous stress-split method of Guenette and Fortin (J Non-Newt. Fluid Mech., 1995). This approach discretizes the Galerkin method for the momentum equation requiring a velocity-pressure space that satisfies the LBB condition, a Petrov-Galerkin method for the constitutive equation, and the addition of a least squares interpolation of the velocity gradient tensor to a continuous space. With the addition of least squares interpolation terms to the momentum equation, the stress space is stabilized. Simulations of this form are computationally demanding, since in addition to the standard Navier-Stokes unknowns, we must also solve a stress tensor and a velocity gradient tensor. Multimode calculations require even more unknowns, adding a stress tensor for each mode. Computational challenges for this problem also include poorly conditioned matrices from the discretization, requiring direct Gaussian elimination methods. A stabilized method has been implemented for time-dependent flows with free and moving boundaries using an arbitrary-Lagrangian-Eulerian method. The method is similar to the Galerkin least squares (GLS) method for the stress equation of Coronado et al. (J Non-Newt. Fluid Mech., 2006), but uses differential, time-dependent forms of the constitutive equations. This GLS form allows for circumvention of the LBB conditions and equal order interpolation of all field variables. The GLS also reduces the condition number of the matrix system, allowing for the use of Krylov-based iterative solvers in place of direct solvers. Two applications will be investigated: deformation of a Newtonian droplet flowing through a constriction surrounded by a viscoelastic fluid and transient blade coating, on a deformable substrate. Both problems require periodic remeshing and remapping as the mesh becomes displaced over time. This GLS implementation will be tested using GMRES with either ILUT or ML as the preconditioner.

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Title: Mechanistically-Based Probabilistic Modeling Compared to Statistical Modeling for Fatigue

Author(s): Gary Harlow, *Lehigh U.*.

Fatigue life prediction historically has been a very challenging problem because mechanistically based models are extremely complex and experimental observation for life exhibit scatter from two to four orders of magnitude. Even so, analyses are typically statistical, and such models do not adequately reflect long-term operating conditions. Yet, in order to certify and qualify a material for an application that requires high reliability for operation and safety, fundamental material properties must be experimentally investigated and validated. The purpose of this presentation is to contrast mechanistically based probability modeling with statistical modeling in fatigue. In order to do this, the well–documented strain–life approach is used as the underlying experimental method for considering the attributes of a primarily statistical approach to modeling fatigue life. Specifically, the variability associated with the median behavior in a strain–life graph for data is examined. The ensuing analyses are based on a substantial database for a cold–rolled, low carbon, extra deep drawing steel; ASTM A969. The statistical distribution function considered for characterizing the fatigue life is a generalized Weibull distribution function that empirically incorporates load history and damage accumulation. The strain–life computation employs the standard Coffin–Manson relationship. In contrast, recent observations of fatigue and associated material observations for SUJ2 steel have shown that that there are distinct physical mechanisms for the nucleation and early growth of fatigue cracks; one associated with surface damage and the other with internal inclusions. Consequently, empirical modeling is insufficient to capture this mechanistic complexity. A simple crack growth based probability model is used to examine plausible contributors to the observed response, e.g., those associated with material properties and manufacturing, which are readily identifiable. A connection between the crack growth model and S–N response, the impact of residual stresses induced by specimen preparation, and the distribution between external and internal nucleation sites are examined. While the analysis is not exhaustive, it indicates the need for mechanistically based probability modeling as opposed to empirically based statistical approaches for fatigue life modeling.

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Title: The SCEC-USGS Dynamic Earthquake Rupture Code Comparison Exercise – Large Earthquake Simulations

Author(s): Ruth Harris, *U.S. Geological Survey*.

I summarize the progress by the Southern California Earthquake Center (SCEC) and U.S. Geological Survey (USGS) Dynamic Earthquake Rupture Code Comparison Group, that examines if the results produced by multiple researchers' earthquake simulation codes agree with each other when computing benchmark scenarios of dynamically propagating earthquake ruptures. These types of computer simulations have no analytical solutions with which to compare, so we use inter-code comparisons to check if they are operating satisfactorily. To date we have tested the codes against benchmark exercises that incorporate a range of features, including single and multiple planar vertical faults, a single planar dipping fault, slip-weakening, rate-state, and thermal pressurization friction, elastic and visco-plastic off-fault behavior, complete stress drops that lead to supershear rupture velocities and extreme ground motion, heterogeneous initial stresses, and heterogeneous material structure. Our most recent benchmarks have involved earthquake rupture simulations that incorporate complexities in fault geometry, and that incorporate heterogeneous velocity structures. Our goal is reproducibility, and we focus on the types of earthquake-simulation assumptions that have been or will be used in studies of earthquake physics or in earthquake hazard estimates. For example, simulations of multi-fault earthquake ruptures help examine the probability of earthquakes being able to cascade among multiple geologic faults which in turn leads to estimates of earthquake size. As another example, the branching fault case and the dipping-fault extreme-ground motion case have both been foci of study due to their potential applications to geologically hazardous settings. Our group's goals are to make sure that when our earthquake-simulation codes simulate these types of earthquake scenarios along with the resulting simulated strong ground shaking, that the codes are operating as expected. For more information about our group and our work, please see our website, scecdata.usc.edu/cvws, and our group's overview papers, Harris et al., Seismological Research Letters, 2009, and Harris et al., Seismological Research Letters, 2011.

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Title: Large Eddy Simulation of Unsteady Combustion Events

Author(s): Venkat Raman, Malik Hassanaly, *U. Michigan*.

Large eddy simulations (LES) have become the standard tool for simulating complex reacting flows, especially in the field of turbulent combustion. Even when chemical reactions are fast and occur at the smallest scales, the ability to capture large scale mixing is seen as a major advantage in the use of LES. This feature allows large-scale information based inputs to the unresolved small-scale models to be more accurate. However, LES appears to be fundamentally limited in its applicability to statistically stationary flows. Following earlier work by Moser and co-workers, it has been established that LES could capture one-time but multi-point statistics. While this limitation has so far not been observed to affect any of the multitudes of configurations that have been studied using LES, the emergence of unsteady or transient flows in engines are testing the applicability of LES. Flame flashback in premixed gas turbines, soot particle generation due to inefficient combustion in aircraft engines, or flame extinction at high altitudes in aircraft and scramjet engines all fall under this class of transient flows attached to consequential failure events. In this talk, the success and limitations of LES in the context of such transient flows will be discussed. Key issues regarding the generation of experimental data for validation will also be discussed. A few examples that illuminate the issue will be used to discuss the range of applicability of LES.

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Title: Molecular Dynamics Simulations of Hydrogen Diffusion and Embrittlement in both BCC and FCC Crystal Structures

Author(s): Mohamed Hamza, Yunes Salman, *British U. Egypt*; Tarek M. Hatem, *British U. Egypt/Max-Planck Inst.*; Jaafar A. El-Awady, *Johns Hopkins U.*; Dierk Raabe, *Max-Planck-Inst.*.

Failure due to Hydrogen Embrittlement (HE) phenomena occurs in many metals and most importantly in high strength steel alloys and nickel based super alloys. A unified understanding of the deformation mechanism of HE has not yet been reached and hence atomic simulations are conducted to study the effect of hydrogen atoms in Bcc iron and Fcc nickel bi-crystals. Grain boundaries (GBs) play an important role in determining the mechanical and physical properties of a material and the structure of GB has an essential role in determining the diffusion and segregation of hydrogen, nucleation and propagation of dislocations. In this study, molecular dynamics simulations are conducted in both alpha-iron and nickel with different GBs configurations in order to investigate the diffusion and segregation characteristics of hydrogen atoms at various conditions. Also loading is applied for hydrogen charged and uncharged models to analyze the hydrogen impact on mechanical properties, nucleation of dislocations and the interaction of hydrogen with existing and generated dislocation networks over time.

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Title: Local and Pointwise Error Estimation Based on the Variational Multi-Scale Theory

Author(s): Guillermo Hauke, Diego Irisarri, *UNIZAR*.

We present a simple explicit method to compute the local and pointwise errors of a given Galerkin finite element solution. The method is based on the Variational Multiscale Theory, where the subgrid scales are modeled with residual-free bubble functions and global Green's functions. One and two-dimensional examples related to the transport equation and elasticity will be shown. REFERENCES T.J.R. Hughes and G. Sangalli. Variational multiscale analysis: the fine-scale Green's function, projection, optimization, localization and stabilized methods, SIAM J. Numer. Anal. 45,539-557, 2007. G. Hauke and M.H Doweidar and M. Miana. The Multiscale approach to error estimation and adaptivity, Comput. Meth. Appl. Mech. Engrng. 195,1573-1593, 2006.

13th U.S. National Congress on Computational Mechanics
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Title: 3D Numerical Modeling with E-FEM Method of Induced Fratures Around Drifts Due to Excavation

Author(s): Paul Hauseux, Jean-Baptiste Colliat, Jian-Fu Shao, *U. Lille1*; Darius Seyedi, *Andra-R&D Division, France*.

3D Numerical simulations of a tunnel excavation 490 meters below ground are presented. An E-FEM method is developped to take into account of cracking and to model the induced fractures around drifts. The level of damage and the extent of the fractured zone vary along drifts and depend on various factors such as the rock properties, in situ stress field, excavation method, etc. A transversely isotropic behaviour is considered for the host rock. Two failure criteria are proposed to characterize tensile and shear fractures: an anisotropic Mohr-Coulomb criterion with a crack opening in Mode II and a Rankine criterion with a crack opening in Mode I. The influence of the anisotropy of rock properties and in situ stress field are mainly studied and discussed.

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Title: Model-Order Reduction for Mesh-Free Analysis of Fracture Problems

Author(s): Qizhi He, Camille Marodon, J.S. Chen, *UC San Diego*.

A framework of model order reduction (MOR) for fracture mechanics using Reproducing Kernel (RK) approximation of the integrated singular basis function method (ISBFM) is proposed. Under ISBFM framework, the near-tip enrichment functions appear only on the boundaries away from the singularity point, allowing a lower order integration scheme for domain quadrature and making MOR for fracture problem easy to construct. Two MOR methods for RK approximated ISBFM systems, the uniform reduction method and the decomposed reduction method, are examined in this study. The decomposed reduction method [1] with separate projections associated with the smooth and non-smooth approximations is capable of preserving the singularity behaviors in the lower-dimensional space. The uniform reduction approach, on the other hand, can yield better conditioning of the discrete system while captures the singular modes if the enrichment functions are properly scaled. The numerical examples are given to validate the effectiveness of the proposed methods. [1] J.-S. Chen, C. Marodon, and H.-Y. Hu, “Model order reduction for meshfree solution of Poisson singularity problems,” Int. J. Numer. Meth. Engng, 2014.

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Title: A Three-Dimensional Full-Eulerian Approach to Fluid-Structure Interaction Problems Using the Level Set Method

Author(s): Ping He, *MIT*; Changwen Mi, *Southeast U.*.

We extended our previously proposed full-Eulerian method, termed solid level set method, to model three-dimensional fluid-structure interaction problems. In this method, each hyperelastic body is represented and tracked using three level set functions, which are X-, Y- and Z-level sets originated from the material coordinates. A static level set function defined on the material coordinates (X, Y, Z) is used to construct the surface of the hyperelastic body from X-, Y- and Z-level sets at any given time. We improved the field extension operations of X-, Y- and Z-level sets on the region outside the hyperelastic body using a reinitialization equation. The strain and stress within a hyperelastic body and the interactions with its surrounding fluids and other contacting hyperelastic bodies are computed using the level set functions and a stress-strain relation, e.g. the neo-Hookean model. A unified momentum equation is utilized to compute one flow field for the entire domain, which enables us to model multiple hyperelastic bodies interacting with each other. The method is suitable for studying a wide range of problems in microfluidics, e.g. printing living mammal cells using ink-jet printers to form functional tissues/organs.

13th U.S. National Congress on Computational Mechanics
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Title: High-Order Adaptive Deforming Mesh Calculations of Silicon Solidification with Kinetics

Author(s): Brian Helenbrook, *Clarkson U.*.

In this research we examine 2D arbitrary-Lagrangian Eulerian simulations of solidification using a adaptive C0 hp-finite element method. An unstructured mesh of triangles is used and is adapted using a Delaunay adaptation method. The Rebay algorithm is used to place the refinement points and different methods of choosing points for removal are investigated. It is shown that the midpoint edge-collapse strategy does not lead to quality meshes but removing the edge point farthest from the center of area of the triangles surrounding the edge marked for removal does lead to quality meshes. This algorithm is then applied to perform high-order simulations of silicon solidification. Solidification kinetics are included following the model of Brandon & Weinstein [1, 2]. This work extends previous spectral element results [3] for the Stefan problem to unstructured meshes so that large changes in the interface shape can be simulated with a high-order accuracy. It is also the first time that a high-order method has been applied to a problem including solidification kinetics. 1. O. Weinstein and S. Brandon. Journal of Crystal Growth, 270(1):232–249, 2004. 2. O. Weinstein and S. Brandon. Journal of Crystal Growth, 268(1):299–319, 2004. 3. E.M. Rønquist and A.T. Patera. International Journal for Numerical Methods in Engineering, 24(12):2273–2299, 1987.

13th U.S. National Congress on Computational Mechanics
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Title: A Reduced-Order Model for an Oscillating Hydrofoil with Large Angles of Attack and Near the Free Surface

Author(s): Dillon Helfers, Rory Kennedy, Yin Lu Young, *U. Michigan*.

Hydrofoils have many applications in the maritime industry. They are utilized in energy harvesting devices, high speed crafts, control surfaces on marine vessels, and they represent simplification of turbines, propellers, as well as many forms of animal locomotion. Since most of these devices operate in spatially and/or temporally varying flows due to body motion, and/or interaction with free surface waves, currents, and adjacent structures, it is necessary to be able to accurately and efficiency predict the unsteady loads, particularly for real time control applications. The focus of this presentation will be on the derivation and validation of a reduced order model (ROM) for the unsteady loads on an oscillating hydrofoil for a wide range of Reynolds numbers, pitch rates, pitch amplitudes, and submergence depths. The model is derived by fitting parametric added mass, damping, and disturbing force terms obtained from time-domain viscous simulations using ANSYS CFX. The results show significant improvements in the accuracy of predictions compared to Theodorsen's analytical potential flow solutions, particularly in the regimes where large scale, vortex shedding where observed, and when the foil operates near the free surface. The results show that while the fluid added mass is independent of speed and frequency, the hydrodynamic damping and disturbing force terms depend on the speed, frequency, and submerged depth. The sign and magnitude of the fluid damping and stiffness terms can deviate substantially from Theodorsen's solution, which can lead to very different prediction of the resonant frequencies and loss factor in water, particularly for lightweight structures operating at high speeds.

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Title: Discrete-Element Bonded-Particle Model of Sea Ice Deformation and Fragmentation

Author(s): Agnieszka Herman, *U. Gdansk*.

Sea ice, permanently or seasonally covering large areas of polar and subpolar oceans, is commonly modeled as a continuum, with various versions of the viscous-plastic rheology. This approach, relatively efficient computationally, gives satisfactory results at large spatial and temporal scales (e.g., the Arctic Ocean), but has important limitations regarding reliable reproduction of certain physical processes, in which the granular nature of sea ice plays a significant role. Until recently, only few attempts to directly account for the granular nature of sea ice have been made ([1-3] and references there). This paper presents the possibilities offered by discrete-element models (DEM) in modeling the dynamics of sea ice and its interactions with surrounding fluids (ocean and atmosphere). The DEM sea ice model used in this work describes the motion and interactions of two types of objects: ‘particles’ (disk-shaped sea-ice blocks moving within a two-dimensional space representing the sea surface) and ‘bonds’ (representing new, usually thinner ice filling open spaces between thicker ice blocks). There are two essentially independent mechanisms of interactions between particles: through direct contact (nonlinear Hertzian contact model, taking into account polydispersity) and through elastic bonds. Numerically, the model is based on the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations) libraries. It consists of a toolbox that enables calculation of external forces acting on the ice (wind, ocean currents, etc.) and sea-ice-specific interactions between the particles and bonds (see [2,3] for earlier model versions). This work concentrates on those aspects of sea ice dynamics that are linked to its extreme polydispersity (power-law floe size distribution). The examples shown illustrate processes that are poorly or not at all reproduced in continuum sea ice models, but are crucial for sea ice dynamics. Although the model has been designed to represent sea ice, the results provide a new insight into the behaviour of other strongly-polydisperse granular materials. REFERENCES [1] R. Gutfraind, S.B. Savage, “Marginal ice zone rheology: Comparison of results from continuum-plastic models and discrete-particle simulations”, J. Geophys. Res., 102, C6, 12647-12661 (1997). [2] A. Herman, “Numerical modeling of force and contact networks in fragmented sea ice”, Annals Glaciology, 54, 114-120 (2013). [3] A. Herman, “Shear-jamming in two-dimensional granular materials with power-law grain-size distribution”, Entropy, 15, 4802-4821 (2013).

13th U.S. National Congress on Computational Mechanics
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Title: Interactive Design Through Parametric Modeling and Isogeometric Analysis of Wind Turbine Blades

Author(s): Austin Herrema, Chenglong Wang, Ming-Chen Hsu, *Iowa State U.*.

This work addresses some practical aspects of making Isogeometric Analysis (IGA) more accessible to design engineers and analysts. While advances in IGA continue to be made in academia, it is still immature in the industrial design context. One of the primary reasons for this is the dissimilarity between methods required to generate analysis-suitable geometries and parametric design paradigms that are standard in industry. This work seeks to propose an accessible, interactive, design-through-analysis platform that takes advantage of both parametric design and IGA. This platform is achieved through several Rhino 3D plug-ins and methodologies: we develop generative algorithms for unique surface models using a visual programming interface for Rhino 3D called Grasshopper 3D, create basic user interfaces for user definition of input parameters, perform mechanical analysis, and visualize the solution fields, all within the same Computer-Aided Design (CAD) program. This design-centric combination of parametric geometry modeling and IGA allows rapid and user-friendly design-through-analysis iteration, and would also serve as an apt vehicle for high fidelity parametric optimization.

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Title: Immersed Fluid-Structure Interaction Strategies for Deformable and Rigid Bodies

Author(s): Christian Hesch, *Karlsruher Inst. Tech.*.

In this talk, we address a most general framework for immersed strategies. In particular, we develop an overlapping domain decomposition method using Lagrange multipliers for the enforcement of congruent velocities in the interacting fields, i.e. the fluid as well as the solid field. A subsequent Null-Space reduction scheme allows us to remove the Lagrange multipliers as well as the redundant coordinates such that we obtain a system with a minimal set of unknowns. The solution for the solid degrees of freedom as well as the Lagrange multipliers, representing a body force field within the fluid, can be carried out easily. This variational consistent framework unifies well-known approaches within the Fictitious Domain (FD) philosophy as introduced by Glowinski. As part of the FD methodology, the Immersed Finite Element Method (IFEM) can be derived from this approach as well. Further improvements of this framework deal with the interpolation of the Lagrange multiplier field. The optimal choice of the underlying shape functions of the multipliers leads to an improvement the overall spatial performance. In a last step, we immerse simultaneously deformable and rigid bodies in a unified manner. Therefore, a specific Cosserat methodology relying on the usage of a director triad for the rigid body kinematic is introduced. This allows us to pass information about the geometrical shape of the rigid body to the fluid. Since the director based formulation relies on a standard finite element mesh, both, deformable and rigid solids can be embedded using the same framework for the body force field.

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Title: Stochastic Sequential Multi-Scale Modeling of Fiber Reinforced Composites

Author(s): Mason Hickman, Prodyot Basu, *Vanderbilt U.*.

In tailoring new materials with desired properties, the deliberate inclusion of fragments of other materials in a matrix is a common approach. A sequential multiscale modeling process can be used to bridge the inclusion scale to the structural scale. A framework for stochastic optimization of materials with engineered microstructures is detailed. Numerical methods for solving problems with short-fiber inclusions are discussed. Addition of fiber reinforcement has been shown to improve the performance of various materials in a number of applications. The behavior of fiber reinforced cementitious materials under tensile stress is dependent on several morphological characteristics. In real-world systems, the distribution of the fibers may be random, with orientation angle and distribution varying locally. The composite material response also depends on the cohesive properties between the fibers and the matrix, which exhibit uncertainty. At the macroscale, modeling to allow for debonding of each individual fiber is not realistic. Even at the representative volume element (RVE) scale it can be difficult to model fiber reinforcement using the finite element method for fiber volume fractions of more than 2%. RVEs are further discretized into statistical volume elements (SVE) whose response is analyzed using the extended finite element method (XFEM). XFEM uses the basic concepts of FEM supplemented with higher-order enrichment functions to capture the effect of discontinuities caused by different phases without the need for a mesh that closely conforms to the material morphology, ideal for specimen with arbitrary fiber distributions. Using a descriptor-based approach, a correlation is assumed between variables that describe the material morphology on the microscale and global material response in the macroscale. The descriptor design space is explored using Latin Hypercube Sampling. Correlation is determined between the descriptor variables and the energy absorption capacity of a fiber reinforced matrix. The variation observed in SVE models is quantified and used for homogenization to bridge the scales of the problem. The macroscale response is modeled using a mesh of pseudo-homogeneous elements with local properties assigned according to the observed material property distributions in SVEs. The performance reliability of macroscale structures with microscale reinforcement is assessed.

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Title: Multiple Time Scales and Pressure Forcing in Discontinuous Galerkin Approximations to Layered Ocean Models

Author(s): Robert Higdon, *Oregon State U.*.

Barotropic-baroclinic time splitting is widely used in ocean circulation modeling to separate the fast and slow motions into distinct subsystems. This talk addresses two aspects of this usage in the context of discontinuous Galerkin (DG) methods. (1) A DG formulation of the pressure forcing requires values of pressure at the cell edges, but the DG representation of pressure may be discontinuous at those edges. In principle, values of pressure at cell edges could be obtained by solving a Riemann problem for the full system, but in a model with many layers this process could be complicated. It is shown here that some ideas related to barotropic-baroclinic splitting can be used to reduce the Riemann problem to a much simpler system of lower dimension. (2) One of the subsystems mentioned above consists of the original governing equations, which are solved in each layer, and the other is a set of vertically-integrated barotropic equations. The barotropic equations are intended to represent fast external motions, and they are solved with a relatively short time step. The layer equations are solved with a relatively long time step that is appropriate for the slow motions in the system, although the layer equations can actually admit both fast and slow motions. The solutions of the two subsystems must continually be made consistent, and a method for enforcing consistency is described here. This method has the unexpected effect of introducing a type of time filtering into the forcing for the layer equations; this appears to explain why those equations can be solved stably with a long time step.

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Title: Coupling Discrete Element Models with Digital Image Correlation Displacement Fields to Simulate Low Temperature Asphalt Concrete Fracture

Author(s): Brian Hill, Oliver Giraldo-Londono, William Buttlar, *U. Illinois*; Glaucio Paulino, *Georgia Inst. Tech.*.

A current research study at the University of Illinois couples heterogeneous discrete element modeling (DEM) with digital imaging correlation (DIC) fields to study the Mode I response of asphalt concrete. DEM particles interact with one another using soft contacts at the micro-scale. In order to capture the macro-scale behavior of asphalt concrete in DEM, the micro-scale contact properties must be defined. Previous research studies defined these properties to match the global load-crack mouth opening displacement (CMOD) response. In addition, researchers previously defined micro-scale properties of heterogeneous asphalt concrete DEM models using elastic contacts in the mastic and aggregate phases. However, improved property calibration is possible through the use of DIC displacement fields, which provide full field measurements of ahead of the notch, and a newly developed DEM mastic phase viscoelastic traction-separation law. The current study employs optimization techniques to match the DIC and DEM displacement fields in addition to the load-CMOD response. This presentation will detail the DEM-DIC coupling technique to systematically determine micro-scale contact properties. Furthermore, the authors will discuss the development of the DEM mastic phase viscoelastic traction-separation law.

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Title: Stable and Efficient Variationally Consistent Nodal Integration for Meshfree Methods Using Taylor Expansion

Author(s): Michael Hillman, J. S. Chen, *UC San Diego*.

Convergent, and stable domain integration that is also efficient remains a challenge for Galerkin meshfree methods. High order quadrature can achieve stability and optimal convergence, but is prohibitively expensive for practical use. On the other hand, low order quadrature such as nodal integration consumes much less CPU, but can yield non-convergent, unstable solutions. Several nodal integration methods have been developed that are convergent and stable [1], but in the end sacrifice much of the efficiency of nodal integration due to the approaches taken to ensure accuracy and stability. In this work, a stabilization scheme for nodal integration is introduced based on Taylor expansion. It is shown that using this method, coercivity of the numerical solution can be increased with a dramatic decrease in cost compared to other common stabilization schemes. Due to the low order quadrature employed, nodal integration schemes necessitate a strategy for achieving optimal convergence. Variational consistency provides a paradigm for attaining optimal convergence of arbitrary order for any given integration scheme [2]. The stabilized nodal integration introduced is formulated in a variationally consistent manner, and it is shown that using this approach, efficiency is still far superior to alternative stable and convergent schemes. Since Taylor expansion requires constructing high order derivatives, which are typically expensive for meshfree methods, implicit gradients [3] are also introduced under the framework to further reduce the cost of the proposed stabilization. Several examples are provided that demonstrate the effectiveness of the proposed method, and efficiency comparisons are made with existing stabilization schemes. References 1. Puso M, Chen JS, Zywicz E, Elmer W. Meshfree and finite element nodal integration methods. International Journal for Numerical Methods in Engineering 2008; 74:416-446. 2. Chen JS, Hillman M, Rüter M. An arbitrary order variationally consistent integration method for Galerkin meshfree methods. International Journal for Numerical Methods in Engineering 2013; 95:387–418. 3. Chi SW, Chen JS, Hu HY, Yang JP. A gradient reproducing kernel collocation method for boundary value problems. International Journal for Numerical Methods in Engineering 2013; 93:1381–1402.

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Title: Modeling Fatigue from Micro-Scale Crack Initiation to Component Failure with Propagated Uncertainty Across Scales

Author(s): Jacob Hochhalter, W. Paul Leser, James Warner, Patrick Leser, Geoff Bomarito, J. Andy Newman, *NASA*.

Autonomous and long duration NASA missions will require the elimination of prohibitive structures and materials design constraints, which are imposed by state-of-the-practice safety assurance methodologies. These constraints stem from a reliance on a wealth of empirical data in an attempt to characterize worst-case scenarios. Furthermore, uncertainty is only accommodated through overly-conservative design and maintenance, rather than reduced. This work focuses on a method for reducing uncertainty in multiscale fatigue modeling by incorporating the digital twin concept, which incorporates as-built component details and in-service usage details to personalize predictions for each aircraft or spacecraft. To test the efficacy of this approach, X-ray computed tomography will be used to gather the sizes and shapes of each of the second phase, crack initiating, particles in a double edge notched specimen. The cracking of each particle will then be predicted [1-4], with uncertainty in their strengths, surrounding grain orientation, and load. The reduction in uncertainty related to the direct measurement of second phase particles, relative to assuming a random distribution, is illustrated. The uncertainty in total fatigue life is then further reduced throughout service life by incorporating usage data and better predictions of load spectra. [1] J. Hochhalter, D. Littlewood, M. Veilleux, J. Bozek, A. Maniatty, A. Rollett, A. Ingraffea (2011) “A Geometric Approach to Modeling Microstructually Small Fatigue Crack Formation: III. Development of a Semi-Empirical Model for Nucleation” Modelling Simul. Mater. Sci. Eng. [2] J. Hochhalter, D. Littlewood, M. Veilleux, J. Bozek, A. Maniatty, A. Ingraffea (2011) “A geometric approach to modeling microstructurally small fatigue crack formation: II. Development of a semi-empirical model for nucleation,” Modelling Simul. Mater. Sci. Eng. [3] J. Emery, J. Hochhalter, P. Wawrzynek, G. Heber, A. Ingraffea (2009) “DDSim: A hierarchical, probabilistic, multiscale damage and durability simulation system – Part I: methodology and Level I,” Engr. Fract. Mech, 76, 9. [4] J. Bozek, J. Hochhalter, M. Veilleux, M. Liu, G. Heber, S. Sintay, A. Rollett, D. Littlewood, A. Maniatty, H. Weiland, R. Christ Jr., J. Payne, G. Welsh, D. Harlow, P. Wawrzynek, A. Ingraffea (2008) “A geometric approach to modeling microstructurally small fatigue crack formation: I. Probabilistic simulation of constituent particle cracking in AA 7075-T651,” Modelling Simul. Mater. Sci. Eng., 16.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Design and Experimental Evaluation of a 3D-Printed Interconnected Microvascular Mimicking Network For Highly Efficient Bone Growth

Author(s): Benjamin Holmes, Michael Plesniak, Lijie Zhang, *George Washington U.*; Kartik Bulusu, *George Washington U.* .

As an emerging tissue/organ manufacturing technique, 3D bioprinting has begun to show great promise in advancing the development of functional tissue/organ replacements [1]. However, one of the biggest current challenges in 3D bioprinted tissues and organs is the need to create a highly efficient 3D perfused vascular network, in cooperation with native cell population recruitment, for adequate host integration. In particular, a vascular network facilitating efficient nutrient transportation and waste removal is essential for cell survival in large tissue systems. Current available strategies for the fabrication of complex vascular networks are extremely limited. Here, we have successfully designed and 3D printed a series of bone scaffolds with microvascular channels, for efficient and enhanced bone growth as well as vascular cell growth. These fabricated polymer scaffolds were coated with nanocrystalline hydroxyapatites (nHA) using a carboxylation process, and evaluated in vitro with human mesenchymal stem cell (MSC) and human umbilical vein endothelial cells (HUVECs). Our results showed that our scaffolds promoted both MSC and HUVEC adhesion with small vascular channels and nHA coatings. Osteogenic differentiation study (calcium and collagen type I depositions) showed that our scaffolds have excellent bone forming potential, in particular for scaffolds with small vascular channels and an nHA coating. Finally, a series of advanced flow mechanics were conducted using an experimental setup designed to replicate pulsatile arterial blood flow and to test scaled up representative models of different bone construct vasculature. Representative models were placed in the straight and curved test sections, and changes in upstream and downstream flow properties were compared to a clean artery control case. It was found that our designed vascular channels do not interfere with pulsatile blood flow, and provide a flow characteristic profile highly comparable to arterial blood flow in normal vascular conditions. Thus, this project has effectively shown that a highly functional vascular-like network can be designed which has highly similar performance properties to native vascular blood flow, and can very effectively enhance bone formation in vitro. [1] Derby B. Printing and prototyping of tissues and scaffolds. Science 2012;338:921-6.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Study on the Design of a Nuclear Battery for Space Missions

Author(s): Jintae Hong, Kwang-Jae Son, Jong-Bum Kim, Young-Rang Uhm, Jin-Joo Kim, *KAERI*.

The Korean government is planning a lunar project to send a spacecraft to the moon in the near future, and many related researches such as a launch vehicle, rover, space antenna, and nuclear battery have been initiated since 2014. Among them, a nuclear battery is one of the most important items for supplying electricity and heat in space. A nuclear battery is a device that generates electric power by using the heat dissipated from radioisotopes. To install a nuclear battery in a spacecraft, it is necessary to solve the optimization problem, i.e., minimizing its weight and maximizing the thermoelectric efficiency. The optimal temperature deviation at both ends of the thermoelectric modules should be maintained to obtain the maximum thermoelectric power while effectively dissipating the heat generated from the isotopes. In addition, radiation shielding and structural robustness for the external shock are also critical issues. First, the available amount of radioisotope and its heat flux were determined according to the load limit. A radiation shield analysis was then carried out to decrease the radiation dose rate up to a safe level. Based on the design of the radioisotope module, FE heat transfer analyses for several design parameters of a nuclear battery were carried out. The initial design concept of the nuclear battery referenced the MMRTG of NASA. The thickness of the heat insulation, shape and alignment of thermoelectric modules, and the design of the cooling fins were optimized from the results of the FE analyses. A structural analysis on the external shock was also carried out to check whether the radioisotope module will be damaged or not. A test mockup using electric power as a heat source was fabricated to check the thermoelectric efficiency, heat loss, workability, and structural safety. The test results of the test mockup showed that the thermoelectric efficiency is less than 1.0% owing to its complex design instead of a low heat flux. Therefore, the design of the nuclear battery was simplified to minimize the heat loss, and FE analyses carried out for the changed design parameters. A new test mockup was fabricated using the simplified design and its performance test was carried out.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Nucleation and the Surface Tension of Dispersed Phases by Molecular Simulation

Author(s): Martin Horsch, *U. Kaiserslautern*.

Computational Molecular Engineering aims at adapting molecular force field methods to the needs of industrial users in process engineering. Only in recent years have sufficently accurate molecular models become available for a wide variety of compounds. By massively parallel high performance computing, molecular dynamics simulation of systems with large numbers of molecules has become a widespread approach for considering processes on microscopic and nanoscopic length and time scales. The results of these simulations yield reliable information on thermodynamic and mechanical properties that can be exported to improve the accuracy of continuum methods. By Gibbs Ensemble or Grand Equilibrium simulation, vapour-liquid equilibria between homogeneous bulk phases can be efficiently sampled. However, in these molecular simulations, the two phases are simulated separately as homogeneous systems, so that no interface is present and interfacial properties cannot be considered. In systems where a phase boundary is present, the relaxation time is longer than for the homogeneous fluid, and the long-range contribution to the intermolecular interactions and the computed thermodynamic properties is more pronounced. A computational approach considering fluids at interfaces needs to take this into account. The present talk addresses molecular simulation of the vapour-liquid surface tension for dispersed phases, i.e. small bubbles and droplets as well as thin films, and the homogeneous nucleation processes that occur in fluids at metastable conditions such as supersaturated vapours and subsaturated liquids under tension. It is shown that efficient simulation methods can contribute to obtaining a precise outcome with a comparably limited effort, and how scale-briding molecular simulations can contribute to quantifying the influence of finite-size effects on thermodynamic properties of fluid interfaces. In a homogeneous nucleation process, nuclei of a dispersed fluid phase, i.e. clusters or cavities, emerge from a metastable phase that surrounds them. Molecular dynamics simulation permits computing the nucleation rate and thermodynamic properties of metastable states which are impossible to reach experimentally. The nucleation processes, which are considered by non-equilibrium simulation, are influenced by the interfacial properties of dispersed phases, which are considered by equilibrium simulation. An analysis of finite-size effects explains why the classical nucleation theory predicts the nucleation rate relatively accurately in certain cases, while it fails by up to 40 orders of magnitude for cavitation in carbon dioxide.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Topology Optimization for Path-Dependent Problems

Author(s): Hiroya Hoshiba, Junji Kato, Kenjiro Terada, Takashi Kyoya, *Tohoku U.*.

This study deals with topology optimization considering path-dependent problems. The procedure of sensitivity analysis for topology optimization must be appropriately formulated depending on design functions, material models and the structure analysis. Under the path dependency typified by elastoplostic behavior, an incremental analysis is performed because the stress-strain relationship cannot be uniquely determined. The common problems here are high computational costs and the difficulty to obtain of accurate sensitivity due to the discontinuous stress-strain behavior. In our previous study [1], we achieved the low-cost and accurate sensitivity analysis using elastoplastic material. In the present paper, we extend it to more realistic nonlinear structural problems and demonstrate the accuracy and performance by a series of numerical examples. [1] J. Kato, H. Hoshiba, S. Takase, K. Terada, T. Kyoya, Analytical sensitivity in topology optimization for elastoplastic composites, Structural and Multidisciplinary Optimization, submitted(2015).

13th U.S. National Congress on Computational Mechanics
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Title: MRI-Based Computational Modeling of Blood Flow and Nanomedicine Deposition in Patients with Peripheral Arterial Disease

Author(s): Shaolie Hossain, *Texas Heart Inst.*; Yongjie Zhang, Xiaoyi Fu, *Carnegie Mellon U.*; Greg Brunner, *Baylor College of Medicine*; Jaykrishna Singh, Paolo Decuzzi, *Houston Methodist Rsch. Inst.*; Thomas Hughes, *UT Austin*.

Peripheral arterial disease (PAD) is generally attributed to the progressive vascular accumulation of lipoproteins and circulating monocytes in the vessel walls leading to the formation of atherosclerotic plaques. This is known to be regulated by the local vascular geometry, hemodynamics, and biophysical conditions. Here, an isogeometric analysis framework is proposed to retrospectively analyze blood flow and vascular deposition of circulating nanoparticles (NPs) in the superficial femoral artery (SFA) of PAD patients. The local geometry of the blood vessel and the hemodynamic conditions are derived from MR imaging, performed before (baseline) and 24 months after stent implantation in the SFA. A dramatic improvement in blood flow dynamics is observed post intervention. A 500% increase in peak flow rate is measured in vivo as a consequence of luminal enlargement. Furthermore, a 32% drop in mean oscillatory shear index (OSI) is observed in silico, indicating reduced disturbed flow post intervention. The same patient information (vascular geometry and blood flow) is then used in a simulation of vascular deposition of systemically injected nanomedicines. NPs targeted to inflammatory cell adhesion molecules including VCAM-1, E-selectin, and ICAM-1 are predicted to preferentially accumulate near the stenosis in the baseline configuration with VCAM-1 providing the highest accumulation (about 1.33 and 1.50 times higher concentration than that of ICAM-1 and E-selectin, respectively). Such selective deposition of NPs within the stenosis could be effectively used for the detection and treatment of plaques forming in the SFA. The presented MRI-based computational protocol can therefore be utilized in analyzing data from clinical trials to study possible correlation between hemodynamics and disease progression (or regression) in PAD patients, as well as to predict the outcome of any intervention, thus providing important insights into disease management.

13th U.S. National Congress on Computational Mechanics
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Title: Simulation of Hydro-Mechanical Behavior of Cementitious Material Using Morphological Model

Author(s): Mahban Sadat Hosseini, Jean-Baptiste Colliat, Nicolas Burlion, *U. Lille1*.

The prediction of deformations induced in cement based materials through time has a great importance for the study of long-term durability of structures and also to extend theirs lifetime. The objective of this work is to develop numerical calculation tools, able to predict the hydro-mechanical behavior of materials such as cement paste. In this simulation the first step is the modeling of the isotherm to characterize hydraulic behavior, and the second step is to evaluate strains induced due to desiccation. A structure during his lifetime faces different relative humidities. Different cycles of drying and saturation impose the fluid transfer in the porous network and the fluid transfer properties are related to the geometrical complexity of the network. This complex structure is characterized by geometric properties associated with the shape (morphology) and the connection (topology) between the pores. Hence a primary objective is to model the microstructure by developing methodologies for topological description of geometry in 3D. The intermediate objective is the modeling of fluid transfer process through the matrix. The morphological simulation is applied on the porous network model in different relative humidity to localize filled and empty pores during intrusion and extrusion. The mathematical tools that were performed in this method are morpho-mathematical operations like erosion, dilation, opening and geodesic reconstruction. As it mentioned, there is no assumption on the pore shape, whereas in most studies the pores are considered as cylindrical or spherical elements. As the result of first part, a numerical sorption – desorption isotherm is obtained and compared with the experimental values. In the following of hydric simulations, the hysteresis between sorption and desorption isotherm is also modeled. In the second part of this study as the final objective, mechanical behavior such as shrinkage due to different cycles of drying and saturation is simulated. To achieve this simulation, the morphological model of cement paste is considered under the effect of capillary pressure and disjoining pressure and the mechanical behavior is modeled using morpho mathematical operations. For example the skeleton is implemented finding the axis of pores to impose forces in right orientation. Considering this, it is possible to apply capillary pressure and disjoining pressure in appropriate and specific places where they are imposed in real complicated porous network. Then the finite element calculation will be executed to obtain shrinkage and it will be compared with experimental values.

13th U.S. National Congress on Computational Mechanics
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Title: Adaptive Discontinuous Galerkin Methods on Polytopic Meshes

Author(s): Paul Houston, *U. Nottingham*.

In this talk we consider high-order/hp-version interior penalty discontinuous Galerkin methods for the discretization of second-order elliptic partial differential equations on general computational meshes consisting of polygonal/polyhedral elements. By admitting such general meshes, this class of methods allows for the approximation of problems posed on computational domains which may contain a huge number of local geometrical features, or micro-structures. While standard numerical methods can be devised for such problems, the computational effort may be extremely high, as the minimal number of elements needed to represent the underlying domain can be very large. In contrast, the minimal dimension of the underlying (composite) finite element space based on general polytopic meshes is independent of the number of geometric features. Here we consider both the a priori and a posteriori error analysis of this class of methods, as well as their application within Schwarz-type domain decomposition preconditioners.

13th U.S. National Congress on Computational Mechanics
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Title: Immersogeometric Analysis with Application to Fluid-Structure Interaction of Heart Valves

Author(s): Ming-Chen Hsu, Michael C. H. Wu, Fei Xu, *Iowa State U.*; Josef Kiendl, *U. Pavia*; David Kamensky, *UT Austin*.

The aim of this work is to develop a geometrically flexible technique for fluid–structure interaction (FSI). The motivating application is the simulation of aortic valve function over the complete cardiac cycle. Due to the complex motion of the heart valve leaflets, the fluid domain undergoes large deformations, including changes of topology. We propose an immersogeometric method that directly analyzes an isogeometric surface representation of the structure by immersing it into a non-boundary-fitted discretization of the surrounding fluid domain. An arbitrary Lagrangian–Eulerian/immersogeometric hybrid methodology is derived under the augmented Lagrangian framework for FSI. A single computation combines a boundary-fitted, deforming-mesh treatment of some fluid–structure interfaces with a non-boundary-fitted treatment of others. This approach enables us to simulate the FSI of a bioprosthetic aortic valve implanted in a flexible artery through the entire cardiac cycle under physiological conditions, demonstrating the effectiveness of the proposed techniques in practical computations. An exponential-type isotropic material model with a Neo–Hookean component will be considered in this work.

13th U.S. National Congress on Computational Mechanics
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Title: An Adaptive Finite-Volume Method for Steady Euler Equations with k-Exact WENO Reconstruction

Author(s): Guanghui Hu, *U. Macau*; Nianyu Yi, *Xiangtan U.*.

In this talk, we will present a general numerical framework of using finite volume method to solve 2D steady Euler equations. The algorithm consists of two iteration methods, i.e., the Newton iteration method which is used to linearize the system, and a geometrical multigrid method which is used to solve the linear system. The k-exact reconstruction is employed to obtain a high order solution representation in each element, and WENO process is introduced to prevent the numerical oscillation around the shock. For the domain with complex geometry, the numerical tests show that our method is not sensitive to the linear approximation for the curved boundary. With the correction of the normal direction for those quadrature points on the curved boundary, our method can handle most cases. The numerical tests show that our method could produce expected high order numerical accuracy, while remove or significantly reduce the nonphysical oscillation successfully. To partially resolve the high demanding on the computational resource for our method, the mesh h-adaption technique is introduced in the algorithm. For the highly efficient mesh management in our h-adaptive method, a hierarchy geometry tree data structure, which is based on the fork-tree structure, is developed. To efficiently generate the reliable error indicator, several possible methods are discussed, including physics based indicator, and goal-oriented a posteriori error estimation based indicator. The numerical tests show that compared with the fixed mesh simulations, our h-adaptive method could effectively improve the efficiency of the simulations. In the last part of this talk, we will give the progress on the work of shape optimal design with our method. This work is a joint work with Prof. Nianyu Yi from Xiangtan University, China.

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Title: Strong and Weak Coupling of Finite Element and Reproducing Kernel Approximations

Author(s): Hsin-Yun Hu, *Tunghai U.*; Jiun-Shyan (JS) Chen, *UC San Diego* .

The coupling of finite element method (FEM) and reproducing kernel particle method (RKPM) has been used for solving complex engineering and scientific problems, such as contact, impact and large deformation problems. The coupling strategy, for example, the relationship between FEM mesh size and RKPM nodal distance and reproducing degree, is an important issue that has not yet been addressed. In this work we introduce two methods for coupling Finite Element and Reproducing Kernel approximations, namely, the weak-weak and the weak-strong coupling formulations. The present work is developed for the static boundary value problems with focus on mathematical analysis. The main results indicate that the weak-strong coupling formulation yields a better convergence and consumes less CPU. The proposed framework can be extended to other meshfree methods coupled with finite element method.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Optimal Sequential Experimental Design Using Dynamic Programming and Transport Maps

Author(s): Xun Huan, Youssef Marzouk, *MIT*.

Experimental data play a crucial role in developing and refining models of physical systems. Data are not all equally useful, however, and some experiments can be more valuable than others. Recognizing that well-chosen experiments can save substantial resources, optimal experimental design seeks to quantify and maximize the value of experimental data. Common current practice for designing a sequence of experiments under uncertainty uses suboptimal approaches: open-loop design that chooses all experiments simultaneously with no feedback of information, or greedy design that optimally selects the next experiment without accounting for future observations and dynamics. By contrast, an optimal sequential design is obtained via closed-loop dynamic programming (DP). This approach accounts for future experiments while making each design decision as late as possible, thus allowing the result of each experiment to guide the design of all remaining future experiments. We use the partially observable Markov decision process (POMDP) variant of dynamic programming, with the goal of acquiring experimental data that are optimal for model parameter inference. We therefore use a design objective that incorporates a measure of information gain. Our approach accommodates nonlinear models and continuous (and often unbounded) parameter, design, and observation spaces. We develop new numerical tools to make solution of the DP design problem computationally feasible. First, transport maps are created to represent belief states, which are the intermediate posterior random variables within the sequential design process. Not only do these maps provide a finite-dimensional representation of these generally non-Gaussian random variables, they also enable fast approximate Bayesian inference, which must be performed millions of times under nested combinations of optimization and Monte Carlo sampling. Second, an adaptive one-step look-ahead value function approximation strategy is used to find the optimal policy. This approximate dynamic programming method iteratively generates scenarios from exploration and exploitation, and uses them to create better approximations of value functions in frequently visited regions of the state space. Finally, various approximation methods are employed to accommodate computationally intensive (PDE-based) models, including polynomial surrogates and stochastic approximation algorithms. These methods are demonstrated on a problem of optimal sequential sensing: inferring contaminant source locations from an airborne sensor in a time-dependent convection-diffusion system, with realistic constraints on aircraft movement and other costs.

13th U.S. National Congress on Computational Mechanics
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Title: A Comparison Study on the Methods of Selecting Rows and Columns in the Adaptive Cross Approximation BEM

Author(s): Shuo Huang, Yijun Liu, *U. Cincinnati*.

In this talk, the results of a comparison study on the adaptive cross approximation (ACA) boundary element method (BEM) will be reported. Specifically, the different methods of selecting the rows and columns of the low rank submatrices in ACA are tested and their efficiencies and accuracies are studied. These different methods include the original method based on the maximum value of coefficients in a column or row, the uniform distribution method, the geometric cross approximation method reported in the literature, and a new gradient based method. Several BEM models, with different geometries and number of elements are tested using the ACA BEM based on the different row-column selection methods. It was found that using the maximum values is still the most effective and efficient method in selecting the rows and columns in the ACA BEM based on the examples studied. Some related issues to the ACA BEM will also be discussed in the talk.

13th U.S. National Congress on Computational Mechanics
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Title: A Mesoscopic Model to Describe Rate-Independent Hysteresis in Filled Rubber

Author(s): Thomas Hudson, Frederic Legoll, Tony Lelievre, *ParisTech*.

In this talk, we present a simple mesoscopic model which attempts to explain a form of rate-independent hysteresis observed in filled rubbers. By passing to a continuum limit, we derive a continuum model which preserves both the evolution of the elastic energy and also the trajectory of the system under cyclic loading.

13th U.S. National Congress on Computational Mechanics
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Title: Advanced Techniques for Coupling Domains for Generalized Solutions Computed by the Proper Generalized Decomposition

Author(s): Antonio Huerta, *U. Politècnica de Catalunya*; Enrique Nadal, Francisco Chinesta, *EC-Nantes*.

Nowadays industries are increasing their interest in the use of composite laminates for their products. Simulations of these fabrication processes imply multi-physics and customized numerical techniques. Traditional techniques such as standard structural finite elements or specially designed shell-type elements are not suitable under this framework because full 3D solutions are required. However, 3D continuum finite elements have a prohibitive cost. Recently, the Proper Generalized Decomposition (PGD) has shown its ability to address these problems in an efficient and accurate manner. PGD is able to obtain 3D solutions at the cost of a 2D computation and it avoids the use of highly distorted or highly refined 3D meshes. However, the PGD-based solvers are not able to deal with complex geometries. Here a novel technique is proposed to cope with complex geometries with a domain decomposition rationale. Thus, splitting the original problem in simplified geometries easily solved with the PGD, a global domain decomposition strategy-like procedure is proposed. Several numerical examples have been presented to show the performance of the method.

13th U.S. National Congress on Computational Mechanics
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Title: An Alternate Approach Towards Synthesis and Analysis of Nonlinear Suspension Kinematics and Dynamics

Author(s): David Kline, Gregory Hulbert, *U. Michigan*.

Towards the development of an automotive suspension synthesis, design and analysis framework, we present the kinematics of suspensions characterized in the context of a kinematic velocity vector (KVV). This KVV concisely tracks changes in the front and side view virtual swing arms, as well as the kinematic ride steer behavior. More formally, the KVV description can be presented via classical screw theory. Results are presented that show that this approach is an appropriate way to characterize the kinematics of a linkage, leading to its application in the automation of suspension geometry generation and analysis. Several examples are provided to demonstrate the efficacy of this screw representation for multi-link suspension systems.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: The Sliding Beam Problem Revisited

Author(s): Alexander Humer, *Johannes Kepler U.*; Loc Vu-Quoc, *U. Florida*.

We present a formulation for the dynamic analysis of sliding beams that are deployed or retrieved through a prismatic joint. The prismatic joint inhibits a transverse deflection and a rotation of the beam's cross-section. As opposed to conventional problems of sliding structures and axially moving continua, we do not assume the beam's axial motion to be prescribed kinematically at the prismatic joint. Being subjected to a possibly large deformation superimposed on the sliding motion, the beam's material points instantly located at the prismatic joint therefore are not known in advance but depend on the structure's current state of deformation. Such kinematic constraint divides the beam into two non-material domains that generally change in the course of motion. Owing to the varying domains, the interface conditions naturally also change over time, which complicates a straightforward solution by means of some numerical method requiring a spatial discretization as, e.g., finite elements. The key idea of the proposed formulation is to circumvent these difficulties by introducing a deformation-dependent transformation of beam's material coordinate, which maps the two varying domains of the structure onto fixed ones. The simpler numerical treatment of the spatial problem enabled by such transformation, however, comes at the cost of a more complex structure of the inertia terms. As usual in the kinematics of relative motion, the material time derivatives of the displacement and the cross-sections' angle of rotation are extended by stiffness and velocity convection terms, whose properties are examined in detail. In the present, more general formulation, the symmetry properties of the matrices obtained upon a Galerkin projection turn out differently from what has previously been discussed in the literature on sliding structures. In addition to the equations of motion based on the geometrically exact theory for planar beams, we present some representative numerical examples, e.g., an extension of the prominent sliding spaghetti problem. By means of these examples, we examine both the behavior of sliding structures and the numerical implications of the proposed approach. For example, we look into distribution and conservation of energy and discuss stability issues of problems of this type. The proposed approach is not limited to sliding beams but can be adopted for closely related problems of axially moving continua and structures with loads moving relatively to it.

13th U.S. National Congress on Computational Mechanics
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Title: Investigation of Deformation Twins Using a DFT-Informed 3D-Phase Field Dislocation Dynamics (PFDD) Model

Author(s): Abigail Hunter, Irene Beyerlein, *Los Alamos Nat'l. Lab.*.

Deformation twinning is a well-known deformation phenomenon in many nanoscale fcc metals. In addition, it is well established that partial dislocations are the basic defect responsible for deformation twins, however the material parameters that control the inclination to twin and the mechanisms that control twin formation are not well understood. Using a density functional theory (DFT) - phase field dislocation dynamics (PFDD) model, we present an unconventional kinetic pathway for twin formation in nanoscale fcc metals that involves two grain boundaries and is active at room temperature and at low strain rates. This work also relates the associated kinetics of nucleation and propagation to intrinsic material defect formation energies. As mentioned, this research uses a 3D PFDD model informed by DFT to investigate the nucleation and propagation of deformation twins at grain boundaries and interfaces in various fcc metals at ambient conditions. The phase field approach is centered on energy minimization and, hence, evolution of the phase field variables and plastic deformation has a direct dependence on system energetics. This is advantageous for investigating extended dislocations and stacking faults because the PFDD model describes these defects using a parameterized gamma-surface (a material dependent energy landscape that describes the energy maxima and minima that atoms must overcome as they shear pass one another on {111} planes) that is developed for specific materials using points from a gamma-surface as simulated by ab initio DFT. This incorporates a dependence on unstable SFEs in addition to the commonly used intrinsic SFE. Additionally, this establishes a link between atomic-scale numerical methods and the DFT-PFDD model that enables us to follow the dynamics of several nucleating and interacting dislocations based on appropriate calculation of their stacking fault widths and accurately probe the physics that underlies plastic deformation of even the smallest volumes.

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Title: An Efficient Binning Scheme with Application to Dynamic Brittle Failure

Author(s): Farah Huq, Lori Graham-Brady, *Johns Hopkins U.*; Rebecca Brannon, *U. Utah*.

The constitutive response of brittle materials under dynamic compression is characterized by the sub-grid-scale crack population enclosed within a typical computational domain, such as a finite element or similar sub-domain. In modeling brittle materials, the macro-scale properties (e.g. elastic compliance) of the material sub-domain is determined by the sampled realizations of the domain's crack population, which varies between elements as a result of natural point-to-point variability in micro-morphology. Since a large number of cracks is expected to be residing within each finite element, it is not practical to track each of their growth and evolution at every time step. Thus an efficient binning scheme is required to predict the representative constitutive response of the large population of discrete cracks. In this research work, a novel binning scheme is developed, which replaces the intractably large crack population by a smaller sub-population of cracks by means of a grid laid out in an unit square probability space. The crack data (e.g. length and orientation for a 2-D problem) is represented by random numbers in the unit square probability space. The data is first mapped to the nodes of the grid in the probability space and then transferred to the Gauss points associated with the grid. The locations of the Gauss points are considered as the bin locations or the representative property of the sub-population of cracks associated with that bin. The weight corresponding to each Gauss point is considered as bin occupancy. To demonstrate the efficiency and accuracy of the approach, the binned crack data with a variety of grid morphologies are used in a micromechanics damage model for brittle materials under dynamic compression. The binned solution using the non-uniform grid with finer discretization in the region of larger cracks matches the exact solution (in which each crack is modeled individually) most accurately. This approach is applicable to different problems that deal with large sets of data since it is generalized by using the probability space. It is also very useful for large-scale simulations as any desired number of bins can be used by manipulating the grid while retaining an acceptable level of solution accuracy.

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Title: Flowgraph Models for the Bayesian analysis of Stochastic Processes

Author(s): Aparna Huzurbazar, *Los Alamos Nat'l. Lab.*.

Stochastic processes, in particular, semi-Markov process (SMP) models, play an important role in the analysis of time-to-event data. SMPs include Markov processes, Markov chains, renewal processes, Markov renewal processes, Poisson processes, birth and death processes, and M/G/1 queues to name a few. They provide a rich framework for many real-world problems. However, in practice, data analysis for SMPs has not been used as widely as one would expect, given their generality. A key reason for this is the perceived complexity of solving semi-Markov models. Many practitioners prefer “simpler” models such as continuous-time Markov chains. We believe that SMPs are extremely flexible and should be the primary statistical tool for uncertainty quantification and modeling of stochastic processes. This talk will introduce statistical flowgraph models (Huzurbazar, 2005) as a tool to bridge the gap from theoretical solutions to practical implementation for uncertainty quantification in complex stochastic processes. In addition to computing first passage time distributions and the probability that the process is in a given state at a given time, we are also interested in estimating the uncertainty associated with these quantities based on uncertainties in estimating transition probabilities and waiting time distributions. This can be done more naturally in a Bayesian setting. Recently, Collins and Warr (2015) demonstrate the theory and computation needed to implement SMP to allow practitioners to use sicher SMP models without being hindered by rigorous mathematical theory. Collins, D. and Warr, R. (2015). A Comprehensive Method for Solving Finite-State Semi-Markov Processes. International Journal of Simulation and Process Modelling, accepted for publication. Huzurbazar, A. (2005). Flowgraph Models for Multistate Time-to-Event Data, NY: John Wiley & Sons.

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Title: An Extended Finite Volume Method for Particulate Flow of Bio-Fluids

Author(s): Susanne Höllbacher, Gabriel Wittum, *U. Frankfurt*.

Summary: A novel X-FV method is introduced to handle particles in viscous bio flows. Main ingredients are using extended velocity spaces and a partition of unity apporach. Abstract: A fully-coupled discretization method for the direct simulation of freely moving particles in fluids is presented. The method is applied to simulate the motion of synaptic vesicles (d=40 nm). Hundreds of these vesicles are floating in small compartments of brain cells. These dynamics are mainly driven by small fluctuations of the surrounding intracellular fluid. Due to viscosity, the hydrodynamic interaction between particles via the surrounding fluid is the key issue. The main question in this context is how the presence of rigid particles with certain size and shape influence the dynamics of the whole system. Since the particles are driven passively by the fluid, a bi-directional fluid-particle momentum coupling has to be handled. The aim of our fully-coupled discretization is to capture this two-way interaction between the fluid and the particles. Our approach is based on extending the ansatz spaces of our finite volume element method, [1], by special functions marking the particles. We avoid introducing additional terms into the continuous fluid equation. Instead, we impose the rigidity constraint by choosing appropriate approximation spaces satisfying rigid body motion in the corresponding domain, as done in [2]. A partition of unity approach helps to formulate the scheme consistently. The extension of the velocity spaces yields two additional unknowns for each particle, the translational and rotational parts of its velocity, respectively. The new system of discrete equations can be completed using that the angular momentum of each particle is preserved. As a result, the fluid velocities are directly coupled with those of the particles in the discretized problem. We verified our method quantitatively by comparison with analytic results for a freely falling particle in two and three dimensions. We also compared our results with data from recent publications. References [1] Nägele, S., Wittum, G.: On the Influence of Different Stabilisation Methods for the Incompressible Navier-Stokes Equations, J Comp Phys, 224(2007)100–116. [2] Wagner, G. J. and Moes, N. and Liu, W. K. and Belytschko, T., The extended finite element method for rigid particles in Stokes flow, IJNME, 51:293-313, 2001

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Title: Array-Based Distributed Modifiable Mesh Structure

Author(s): Dan Ibanez, Mark Shephard, *RPI*.

Over the years a number of investigators have proposed alternative structures for the representation of unstructured meshes. A key reason for the introduction for a number of alternatives is the trade-off between compactness of the representation and its ability to support a variety of operations as needed by applications ranging from providing low order analysis programs with just basic connectivity information to support the mesh generation requirement of high order methods using curved geometry mesh entities. In this presentation we will discuss recent work on a new array-based distributed mesh data structure being developed to support full simulation workflows on massively parallel computers. The workflows to be supported start from a general problem definition in terms of a high level geometry (e.g., CAD model) and include mesh generation, mesh adaptation and all unstructured mesh analysis requirements. The distributed mesh data structure to be presented efficiently supports local modification and migration of elements between parts in a parallel mesh partition. The entire structure is stored in a few large arrays, bringing the benefits of compactness and ease of implementation together with the ability to quickly make modifications. This is the first structure to combine compact array storage with a fully general mesh modification capability. Our structure is a topological representation of the mesh, and focuses on encoding the topological adjacency graph of a mesh. It is flexible enough to allow many variations of adjacent storage schemes, including full and reduced representations. A predefined number of different element types can coexist in the same mesh. The parallel inter-part connectivity is also stored in arrays, and allows choices about which entities to link between parts and how. The key aspect of the inter-part links is their scalability, which strictly binds memory use by the number of neighbors times the number of boundary entities. By avoiding any dependence on the total part count, this structure scales to fill leadership-class supercomputers.

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Title: Why Particle Methods Can Go Faster than Classical FEM to Solve Convective-Dominant Problems?

Author(s): Sergio Idelsohn, *ICREA*; Eugenio Oñate, Julio Marti, Pablo Becker, *CIMNE*; Norberto Nigro, Juan Gimenez, *CIMEC*.

One of the main drawbacks of all the time integration algorithms using an Eulerian formulations is the restricted time-step to be used to have acceptable results. For the case of the Navier-Stoke equations it is well known that in the explicit integrations, the time-step to be used in the solution is stable only for time-step smaller than two critical values: the Courant-Friedrichs-Lewy (CFL) number and the Fourier number.. Both numbers must be less than one to have stable algorithms. For convective-dominant problems like medium and high Reynolds number flows, the condition CFL<1 becomes crucial and limit the use of explicit methods or outdistance its to be efficient. On the other hand, implicit integrations using Eulerian formulations are restricted in the time-step size due to the lack of convergence of the convective non-linear terms. Both time integrations, explicit or implicit are, in most cases, limited to small CFL numbers. The cases in which the problem to be solved include free-surfaces or moving internal interfaces, like multi-fluids of fluid-structure interactions this time-step limitation is even worse. The objective of this presentation is to demonstrate why the method called PFEM-2 based on particles that move in a Lagrangian frame is faster than a classical Eulerian FEM in certain particular cases when large time-step and/or coarse meshes are used. The authors claim that nowadays, the best way to improve the efficiency of the majority of the CFD problems is the use of this particle-based method.

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Title: New High-Order Accurate Isogeometric Elements with Reduced Dispersion for Wave Propagation Problems

Author(s): Alexander Idesman, *Texas Tech U.*.

There are the following issues with existing numerical methods for wave propagation problems: a) a large dispersion error of space-discretization methods may lead to a great error in space; b) due to spurious high-frequency oscillations, the lack of reliable numerical techniques that yield an accurate solution of wave propagation in solids; c) the treatment of the error accumulation for long-term integration; d) the increase in accuracy and the reduction of computation time for real-world dynamic problems. A new numerical approach for computer simulation of the dynamic response of linear elastic structures is suggested. The new technique is very general, and would be of equal value in such diverse applications as: earthquakes; elastic and acoustic wave propagation; crashes; dynamics testing of aerospace vehicles, airplanes, bridges and buildings; and others. The new approach, which resolves the issues listed, includes two main components: a) a new dispersion reduction technique for linear and high-order isogeometric elements, and b) a new two-stage time-integration technique which includes a new two-stage solution strategy with the stage of basic computations and the filtering stage, a new exact analytical a-priori error estimator in time for second- and high-order methods; and a new calibration procedure for the quantification and filtering of spurious oscillations; new criteria for the selection of time-integration methods for elastodynamics. In contrast to existing approaches, the new technique does not require guesswork for the selection of numerical dissipation and does not require interaction between users and computer codes for the suppression of spurious high-frequency oscillations. We should also mention the efficiency of the new high-order isogeometric elements with reduced dispersion. The order of the numerical dispersion error is reduced by a factor of two compared with the conventional isogeometric elements and correspond to the 8th and 12th orders for quadratic and cubic elements, respectively. The new technique also reduces the dispersion error for the lumped mass matrix to the 4th and 6th orders for quadratic and cubic elements, respectively. Numerical examples show that the new approach yields an accurate non-oscillatory solution for impact and wave propagation problems and considerably reduces the number of degrees of freedom and the computation time in comparison with existing methods. Using the new approach, wave propagation and structural dynamics problems are uniformly solved.

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Title: Computational Study of Airway Closure and Reopening in Crackle Lung Sounds

Author(s): Satoshi Ii, Shigeo Wada, *Osaka U.*.

Crackle sound occurs during breathing in a distal small airway with a diameter about 0.5mm, called terminal bronchiole or respiratory bronchiole. Since a mucus thin film is lined in the airway lumen, the airway partially undergoes closures with forming liquid bridges in a deep expiration or normal expiration but with rich mucus in pulmonary disorders, e.g., pneumonedema. And then, during inspiration, the closed airway is suddenly open as a pleural pressure negatively increases. Although this airway motion highly relates to the crackle sounds, the transient mechanism from the airway dynamics to the sound generation and propagation has not been uncovered yet. Some experiment, theoretical and computational studies have tackled this problem and speculated on the mechanism, although a clear consensus has never been codified due to complexity of the problem involving many multicomponent physics: airway wall deformation; mucus motion; fluid motion; acoustic fluctuation. Recently, a fully Eulerian fluid-solid coupled model (Sugiyama et al., 2010, 2011) has been proposed for a suspension flow with deformable solids. In this method, all the material components are expressed by using phase functions and all the physical equations are completely discretized on a fixed mesh based on a mixture formulation. Thus, the explicit representation of the individual components is unnecessary, inferring the multicomponent mechanics are naturally incorporated into a physical model with a monolithic approach. In this study, to uncover the transient mechanism between airway dynamics and sound generation, the monolithic numerical model is newly developed for the crackle sounds by applying the fully Eulerian coupled model for the dynamics of solid deformation, liquid surface tension, fluid motion, material compressibility and acoustic propagation. By simulating the airway closure and reopening, we will find out which dynamics mainly contributes to the acoustic fluctuation in the crackle sounds.

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Title: Proper and Smooth Orthogonal Decomposition-Based, Model-Order Reduction for Complex Systems

Author(s): Shahab Ilbeigi, David Chelidze, *U. Rhode Island*.

Abstract: Computation time is a major issue in numerical simulations of large-scale models of complex dynamical systems [1]. High fidelity reduced order models (ROMs) can be used to overcome these issues, but are hard to develop and test [2]. In a recent study [2], model order reduction of a nonlinear Euler-Bernoulli beam as a complex geometrically nonlinear system has been investigated. Linear subspaces which were spanned by bases from Proper Orthogonal Decomposition (POD) and Smooth Orthogonal Decomposition (SOD) were used to obtain the ROMs. Although it was shown that SOD outperformed POD, both methods were unable to provide lower order representation of full scale models which could be due to either numerical instability of the used explicit space-time method or weak couplings between axial and transverse vibrations of the beam. In the present study, the system under investigation is a grid of masses which are connected by springs and dampers. This system, when subjected to transverse dynamic loading, has geometrical nonlinearity which is caused by the week coupling between axial and transverse vibrations of the masses. However, unlike nonlinear Euler-Bernoulli beam, full state-space model of the system can be obtained analytically and then solved by an appropriate implicit scheme. This clarifies how the week coupling affects the obtained ROM. In order to identify low dimensional POD- and SOD-based ROMs, the recently developed concepts of dynamic consistency and subspace robustness have been used [3]. Results from POD and SOD are then discussed and contrasted. References: [1] Stadlmayr, D., Witteveen, W., "Model Reduction for Nonlinear Multibody Systems Based on Proper Orthogonal- & Smooth Orthogonal Decomposition." Proceedings of IMAC XXXIII, A Conference on Structural Dynamics, 2015. [2] Ilbeigi, S., Chelidze D. "Model Order Reduction of Nonlinear Euler-Bernoulli Beam." Proceedings of IMAC XXXIII, A Conference on Structural Dynamics, 2015. [3] Chelidze, D. "Identifying Robust Subspaces for Dynamically Consistent Reduced-Order Models." Nonlinear Dynamics, 2, 123-130. 2014.

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Title: Viscosity Reduction in Bimodal Suspensions of Two Types of Capsules

Author(s): Yohsuke Imai, Hiroki Ito, Daiki Matsunaga, Toshihiro Omori, Takami Yamaguchi, Takuji Ishikawa, *Tohoku U.*.

Blood is a suspension of different types of capsules, red blood cells, leukocytes, and platelets. We numerically investigate the rheology of bimodal suspensions of two types of capsules. The boundary element method for Stokes flows with a multipole expansion technique is coupled with the finite element method for membrane mechanics, and all procedures are fully implemented in graphics processing unit computing. Our results demonstrate that the shear viscosity of bimodal capsule suspensions is reduced compared to that of monomodal suspensions. We also present the relationship between the viscosity reduction and the deformation and orientation of capsules.

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Title: Reduced-Order Modeling for Highly Dense Heterogeneous Materials

Author(s): Axinte Ionita, Matthew W. Lewis, *Los Alamos Nat'l. Lab.*.

Highly dense heterogeneous materials (HDM) are composite material systems with high filled particle volume fraction and constituents that are described by complex constitutive models (rate and temperature dependence, complex damage behavior, etc.). In the present work HDM are modeled using a Representative Volume Element (RVE) obtained from 3D Computed Tomography (CT) based on the image of a real material. The constitutive laws for the components of the RVE are calibrated from experimental data. Using Direct Numerical Simulations (DNS) applied on the HDM-RVE model one develop a Reduced Order Modeling (ROM) for the HDM systems. The ROM allows to identify the deformation and failure mechanisms of the HDM systems and can be included in multiscale complex numerical simulations.

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Title: On the Construction of Mesh-Free, Finite-Volume Particle Methods for High-Order Numerical Flow Simulation

Author(s): Armin Iske, *U. Hamburg*.

This contribution discusses the construction of meshfree kernel-based adaptive particle methods for high order numerical flow simulation, where the finite volume particle method (FVPM) is used as a prototype. In the FVPM, scattered data approximation algorithms are required in the recovery step of the WENO reconstruction. We first show how kernel-based approximation methods can be used to obtain WENO reconstruction schemes of arbitrary order, before we discuss important aspects concerning the numerical stability and approximation behaviour of polyharmonic spline kernels. Moreover, we propose customized coarsening and refinement rules for the adaptive resampling of the particles. Supporting numerical examples and comparisons with other radial kernels are finally provided.

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Title: A 3D Anisotropic Diffusion Scheme for Laser Plasma Interaction on ALE-AMR Meshes

Author(s): Pascal Jacq, Jerome Breil, *CELIA*.

In the context of High Energy Density Physics (HEDP) and more precisely in the field of laser plasma interaction, Lagrangian schemes are commonly used. The lack of robustness due to strong grid deformations requires the regularization of the mesh through the use of Arbitrary Lagrangian Eulerian (ALE) methods. Theses methods usually add some diffusion and a loss of precision is observed. In this talk we propose to use Adaptative Mesh Refinement (AMR) techniques to recover this loss of accuracy. We will focus our presentation on the resolution of the anisotropic diffusion operator on ALE-AMR grids. The scheme obtained is an extension of the CCLADNS [1] scheme in 3D [2] which is able to handle this kind of meshes. [1] A nominally second-order accurate finite volume cell-centered scheme for anisotropic diffusion on two-dimensional unstructured grids, P.-H. Maire, J. Breil, Journal of Computational Physics, Volume 231, Issue 5, Pages 2259-2299 (2012) [2] A nominally second-order cell-centered finite volume scheme for simulating three-dimensional anisotropic diffusion equations on unstructured grids, P. Jacq, P.-H. Maire, R. Abgrall, Communications in Computational Physics, Volume 16, Issue 4, Pages 841-891 (2014)

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Title: Strategies for Mesh Adaptivity in the Context of Bayesian Inverse Problems

Author(s): Jayanth Jagalur Mohan, Youssef Marzouk, *MIT*.

Formulating an inverse problem in the Bayesian framework allows one to quantify uncertainty in a mathematically rigorous manner. Therein, prior knowledge of the parameters to be inferred, given data, and models that relate parameters to the data are combined using Bayes' rule to provide a revised posterior estimate for the parameters. In the context of physical problems the models are often partial differential equations (PDEs), with the parameters to be inferred being unknown spatial random fields or locations of sources that drive the problem. Typically the task of solving PDEs is addressed by numerical methods such as the finite element method, thus requiring a mesh. Adaptively building meshes that help achieve a satisfactory solution is essential in order to reduce computational overhead. The topic of error estimation and adaptivity has been explored extensively for deterministic forward problems and continues to be an active research field. In the context of Bayesian inversion, one encounters additional complexities during the task of error estimation and adaptivity. The parameters being inferred also implicitly define the PDE or the model. A mesh that may work well for one instance of the parameters may not be suitable for another instance. It is thus desirable to obtain a mesh that can reduce the numerical error to a specified tolerance either for all possible instances of the parameters--or, more practically, for parameter values in high-probability regions of the posterior. We formalize this problem by developing posterior-focused error estimates and adaptivity criteria that build on adaptive procedures for deterministic inverse problems. We make the link between the deterministic and Bayesian settings with the help of variational approaches, such as the randomize-then-optimize (RTO) algorithm, for posterior sampling.

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Title: Review of Recent Developments and Challenges in CFD Modeling of Vortex-Induced Vibrations and Flapping Dynamics

Author(s): Rajeev Jaiman, *Nat'l. U. Singapore*.

In the dynamics of coupled fluid-structure interaction, the phenomenon of frequency lock-in occurs for a given range of control parameters and the frequency of the one system (e.g., fluid wake) deviates from its expected values while being close the value of frequency of the another system (e.g., vibrating/flapping structure). It constitutes an interesting problem for the numerical and mathematical modeling and can cause significant problems for systems used in aerospace, ocean, and offshore engineering, including cables, moorings, risers, subsea pipelines and large floating structures. Oscillating cylinder laterally or flapping of flexible foils in a free stream can form a great variety of vortex wake modes that have a profound role on the performance of structural dynamics. In the case of vortex-induced vibration, the frequency of unstable wake system approaches that of the oscillating bluff body that results into the oscillating lift force with increasing amplitude of motion through a resonance shift. For sufficiently large amplitude, the wake is significantly perturbed and forced to move through the inertial coupling at the natural resonating frequency of the oscillating structure. The extent of lock-in, in terms of reduced velocity, is known to be significantly affected by the mass ratio between the structure and fluid systems. We review recent CFD developments in this interesting topic, and we draw some parallels between vortex-induced vibration and flapping dynamics as a dynamic equilibrium between the instability of the flow and the resonant response of structures. We shed light on the effects of the mass ratio, Reynolds number, reduced velocity, and near-wall proximity. Finally, we provide a review of challenging problems that keep intense interest on the topic.

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Title: Multi-Variate Weighted Leja Sequences for Polynomial Approximation and UQ

Author(s): John Jakeman, *Sandia Nat'l. Labs.*; Akil Narayan, *U. MA Dartmouth*.

Polynomial chaos expansions (PCE) have become a popular and efficient means of building surrogates of high-fidelity simulation models. Much research has been devoted to building PCE for uniform variables, however less attention has been given to constructing approximations in non-uniform (weighted spaces). Sparse grids are popular for PCE in high-dimensions, however these approximations are built on sample sets which are often only very weakly nested and have poor granularity, i.e a jump for one level to the next requires many samples. In this talk we present a novel method for constructing Leja sequences for polynomial interpolation in weighted probability spaces. The sequences are completely nested and have the finest possible granularity. An important feature of Leja sequences is that they are constructed one at a time and the resulting samples concentrated in regions of high probability, which makes Leja sequences ideal for conducting UQ with a fixed simulation budget. To demonstrate the efficacy of the proposed method we present a number of theoretical and numerical results.

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Title: Topology Optimization of Structures with Viscoelastic Creep Constraints

Author(s): Kai James, Haim Waisman, *Columbia U.*.

Topological design of inelastic and non-linear materials is a growing area of interest within the structural optimization community, since linear elastic models are unreliable for large classes of engineering materials and structures. Several studies have investigated structural design while accounting for viscoelasticity in the context of damping and fluid-structure interaction, however very few authors have explored viscoelastic creep deformation due to sustained loading. The current research presents a mathematical framework for generating optimal structural designs while accounting for creep deformation. We have implemented a linear viscoelastic finite element model, and derived the corresponding time-dependent adjoint sensitivity formulation. The resulting analysis models were then incorporated into a computational topology optimization framework in order to achieve optimal topologies based on the target lifespan or operating cycle of the structure. Designs were optimized for minimum mass subject to a constraint on the maximum creep deflection. The method was tested via a series of two-dimensional numerical examples that include design-dependent gravitational loading (self-weight) and time-dependent applied loads. Creep plots are used to quantify the impact of the viscoelastic optimization method as compared with a conventional linear elastic approach. Results show that the design of the optimal structure is highly dependent on the load duration and the complete load history. This observation validates the design premise that it is necessary to account for the full load history and viscoelastic response of the structure in order to achieve optimal long-term performance.

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Title: Modeling Crack Propagation Under Extreme Loading in Mindlin-Reissner Shells Using X-FEM

Author(s): Yannick Jan, Thomas Elguedj, Alain Combescure, *INSA-Lyon* ; Bruno Leblé, *DCNS Rsch.*.

In shipbuilding industry, classical methods to analyze the behavior of structures under extreme loadings are very dependent on the size of the mesh. Moreover, propagation over long lengths with volumetric models requires huge processing power, often inaccessible within this framework. In order to manage these issues and du to the geometry to be considered, a coupling between shell finite element and the extended finite element method (X-FEM) using an adapted propagation criterion is proposed. The developments are made in the fast explicit dynamic finite element code EUROPLEXUS, CEA Saclay. For shell structures involving significant thickness such as submarines, Mindlin-Reissner theory is needed to enable shear strain. Therefore, locking-free element are used to avoid the numerical issue of shear-locking that appears when the shell becomes too thin. The fracture of Mindlin-Reissner plates based on the X-FEM discrete approximation framework is studied by Dolbow and Belytschko [1] with the MITC4. A four node shell element using the same formulation is here only enriched with a step function along the crack line to take into consideration the discontinuity of the displacement field across the crack. The calculation remains accurate without the asymptotic enrichment functions near the crack-tip, as long as the mesh is refined near the crack tip. The numerical integration issue for elements cut by the crack is solved by a partitioning strategy developed by Elguedj [2]. Since the crack is contained in the shell for which the mid plane's position is entirely known, only one information left is needed to locate it. Therefore, a crack is represented by several line segments on the three-dimensional mesh. Only through thickness cracks are considered so far. As regards to the crack propagation, a local criteria proposed by Haboussa [3] is used based on the calculation of mechanical equivalent quantities in the vicinity of the crack tip. The maximum of the equivalent stress tensor near the crack tip is used to decide if the crack propagates as well as its propagation direction, and the Kaninen equation gives the crack velocity. [1] J. Dolbow et al., « Modeling fracture in Mindlin-Reissner plates with the extended finite element method.», International Journal of Solids and Structures, 2005. [2] T. Elguedj et al., « Appropriate extended functions for X-FEM simulation of plastic fracture mechanics. », Computer Methods in Applied Mechanics Engineering, 2006. [3] D. Haboussa et al., « Simulation of the shear-tensile mode transition on dynamic crack propagations. » International journal of fracture, 2012.

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Title: Optimally Blended Finite-Spectral Element Scheme for High Wavenumber Vibroacoustics

Author(s): Michael Jandron, *Naval Rsch. Lab.*; Jeffrey Cipolla, *Weidlinger Associates, Inc.*; Mark Ainsworth, *Brown U.*.

Minimizing the dispersion error in the numerical solution of vibroacoustic finite element problems at large wavenumbers is vital for high accuracy results. This is especially important for very large models that require many degrees of freedom to resolve these wavenumbers, and hence the computational cost can be significant. Dispersion typically increases as the wavenumbers increase and depends on the order of the interpolation and the numerical integration scheme as well. A motivation of this work is that reductions in computational cost can be obtained if one can relax the “ten node per wavelength” criterion and instead use fewer degrees of freedom to provide the same accuracy. Several authors have proposed ideas in the past to reduce dispersion, but many of these methods require an increase in computational cost which is rather unattractive. We have extended a method proposed by Ainsworth [SIAM J. Numer. Anal., Vol. 48, No.1, pp. 346-371, April 2010] who provided an explicit construction for the weights and integration points of this non-standard quadrature scheme by demonstrating its use in the commercial finite element code Abaqus. Several user defined element (UEL) subroutines have been developed in Abaqus for this purpose. We show that by using this reduced integration quadrature scheme for the mass matrix, in combination with a full or reduced Gaussian integration scheme for the stiffness matrix, reduced dispersion is observed. We have implemented various order 1D, 2D, and 3D finite elements as well as an Euler-Bernoulli cubic Hermite beam. In addition, we demonstrate that the rotational inertias of the C1-smoothness beams can be accurately calculated using the blended quadrature scheme. In this paper, we will discuss the implementation of this method and the improved dispersion results obtained. We will also discuss future avenues of this research.

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Title: Modeling Strategies of Active Flow Control Applied to a Realistic Wing Design

Author(s): K.E. Jansen, *U. Colorado-Boulder*; M. Rasquin, *Argonne Nat'l. Lab./U. Colorado-Boulder*.

Virtual shaping for flight control of aerial vehicles is investigated in this work, where aerodynamics performance of conventional control surfaces such as rudder and flaps can be improved over a wide range of operating conditions [1]. In particular, a series of numerical flow simulations of a realistic vertical tail of a commercial aircraft, with a tapered swept stabilizer and a rudder, is considered. For such configurations, active flow control is known to have the capacity to augment the streamwise momentum near the rudder suction peak near where separation is typically observed to limit rudder effectiveness for high deflection angles. Specifically, we use three different modeling approaches to study the interaction of a cross flow with respectively a single jet and an array of 12 jets. The first and most expensive approach uses Delayed Detached Eddy Simulations (DDES) to model periodic cycles of synthetic jets time-accurately. This approach offers insight into the fundamental physics of the flow structures in the vicinity of the synthetic jet(s) by accurately resolving the complete synthetic jet pathway and the vorticity plume. Excellent agreements have been found between this approach and available experiment data. Similarly, the second approach uses a RANS-SA model to model the periodic synthetic jet cycles. This approach requires about half the number of time steps with respect to DDES for statistical convergence of the mean flow but at the cost of an alteration of the agreement with the experiments. Finally the third approach considers steady blowing jets with RANS-SA. This modeling strategy leads to faster statistical convergence of the resulting mean flow. However, the physics of steady blowing jets is altered with respect to their unsteady counterpart and compared to the two previous approaches. For these simulations, a massively parallel fully implicit stabilized finite element flow solver called PHASTA is used to solve the transient, incompressible Navier-Stokes equations. Two unique assets characterize this flow solver: (i) its ability to perform anisotropic adaptivity of the initial 3D unstructured finite element mesh, and (ii) its strong scaling performance, as it has been shown to scale up to 768k cores of a Blue Gene/Q supercomputer [2]. References: [1] O. Sahni et al. Three-dimensional interactions between a finite-span synthetic jet and a crossflow. Journal of Fluid Mechanics, 671:254-287, 2011. [2] M. Rasquin et al. Scalable implicit flow solver for realistic wing simulations with flow control. Computing in Science and Engineering, 16(6):13-21, 2014.

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Title: Computational Aspects of Growth-Induced Instabilities

Author(s): Ali Javili, Mona Eskandari, Berkin Dortdivanlioglu, Ellen Kuhl, Christian Linder, *Stanford U.*.

The objective of this presentation is to establish a computational framework based on the finite element method to study growth-induced instabilities of bi-layered systems. The bi-layered system consists of a thin growing film on a compliant substrate and this family of problems is of particular relevance to biological systems including biofilms and human airways. The growth of the film can form wrinkling or other more complicated patterns on the surface, overall referred to as growth-induced instabilities, depending on the specific geometry and the boundary conditions of the problem. The underlying continuum mechanics model is based on the multiplicative decomposition of the deformation gradient into its elastic and growth parts. This study elaborates on different methods as well as different finite element types. When comparing the numerical solution against the analytical solutions for simple problems, we observed that eigenvalue analysis provides the most accurate and reliable results. We show that a careful perturbation analysis can also provide satisfactory results if the elements are chosen properly and the perturbation is applied correctly. In addition, to the type of analysis, the film thickness, the growth rate, and the elasticity modulus ratio of the film to the substrate affect the onset of the instability and the wavelength.These findings demonstrate the importance of a correct and reliable numerical scheme. Most technical and biological applications deal with extremely thin growing films that are only a few nano-meters thick. To capture the response of the material in the zero-thickness limit, we adapt the surface elasticity theory of Gurtin-Murdoch and establish an appropriate surface growth model. We demonstrate that surface elasticity is extremely useful and efficient concept to capture certain features of growth-induced instabilities. Our results suggest that the theory of surface elasticity can accurately predict the critical growth for the onset of instabilities. However, due to the intrinsic zero-thickness assumption, it cannot predict the failure mode, unless additional regularization techniques are introduced.

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Title: Effects of Atomic-Scale Structure on the Fracture Properties of Amorphous Carbon – Carbon Nanotube Composites

Author(s): Benjamin Jensen, Kristopher Wise, *NASA*; Gregory Odegard, *Michigan Tech'l. U.*.

The fracture of carbon materials is a complex process, the understanding of which is critical to the development of next generation high performance materials. While quantum mechanical (QM) calculations are the most accurate way to model fracture, the fracture behavior of many carbon-based composite engineering materials, such as carbon nanotube (CNT) composites, is a multi-scale process that occurs on time and length scales beyond the practical limitations of QM methods. The Reax Force Field (ReaxFF) is capable of predicting mechanical properties involving strong deformation, bond breaking and bond formation in the classical molecular dynamics framework. This has been achieved by adding to the potential energy function a bond-order term that varies continuously with distance. The use of an empirical bond order potential, such as ReaxFF, enables the simulation of failure in molecular systems that are several orders of magnitude larger than would be possible in QM techniques. In this work, the fracture behavior of an amorphous carbon (AC) matrix reinforced with CNTs was modeled using molecular dynamics with the ReaxFF reactive forcefield. Care was taken to select the appropriate simulation parameters, which can be different from those required when using traditional fixed-bond force fields. The effect of CNT arrangement was investigated with three systems: a single-wall nanotube (SWNT) array, a multi-wall nanotube (MWNT) array, and a SWNT bundle system. For each arrangement, covalent bonds are added between the CNTs and AC, with crosslink fractions ranging from 0-25% of the interfacial CNT atoms. The SWNT and MWNT array systems represent ideal cases with evenly spaced CNTs; the SWNT bundle system represents a more realistic case because, in practice, van der Waals interactions lead to the agglomeration of CNTs into bundles. The simulation results will serve as guidance in setting experimental processing conditions to optimize the mechanical properties of CNT composites.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Modeling Large Deformation with Coupled Eulerian-Lagrangian Technology in Abaqus

Author(s): Huidi Ji, *Simulia* .

In this talk we will give an overview of the coupled Eulerian-Lagrangian technology in Abaqus. With this approach the fluid is modeled with Eulerian elements, and the coupling between the fluid and structure is implemented through contact. This approach was implemented in Abaqus/Explicit with additional features such as mesh motion, adaptive mesh refinement and tracer particles. In addition to modeling FSI problems, this approach is also extremely useful when modeling solids with large deformation. We will present examples such as blast loading, tank sloshing, metal forming and etc. References: 1. Benson, D. J., “Computational Methods in Lagrangian and Eulerian Hydrocodes,” Computer Methods in Applied Mechanics and Engineering, vol. 99, pp. 235–394, 1992. 2. Benson, D. J., “Contact in a Multi-Material Eulerian Finite Element Formulation,” Computer Methods in Applied Mechanics and Engineering, vol. 193, pp. 4277–4298, 2004. 3. Peery, J. S., and D. E. Carroll, “Multi-Material ALE methods in Unstructured Grids,” Computer Methods in Applied Mechanics and Engineering, vol. 187, pp. 591–619, 2000.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Modeling the Evolution of Microdomains on Three-Dimensional Giant Unilamellar Vesicles with a Phase-Field Approach

Author(s): Wen Jiang, John Dolbow, *Duke U.*; Anand Embar, *Dassault Syst. Simulia Corp.*; Eliot Fried, *Okinawa Inst. Sci. & Tech.*.

ABSTRACT A chemo-mechanical model[1] is used to capture the formation and evolution of microdomains on the deforming surface of giant unilamellar vesicles (GUVs). The GUV is assumed to consist of a binary mixture of lipid species. The chemical energy is characterized by a Cahn–Hilliard type density functional that characterizes the line energy between domains of different species. The generalized Canham–Helfrich–Evans model provides a description of the mechanical energy of the vesicle membrane. A key aspect of the chemo-mechanical model lies in its focus on capturing the distinct difference in time scales between shape deformation and phase evolution. This is achieved by ensuring that mechanical balance continues to hold away from chemical equilibrium. The model is cast in a phase-field framework, thus facilitating a diffuse interface approximation of the vesicle surface and the lipid components on the surface. The resulting fourth-order non-linear system of equations is discretized using the spline-based finite element method. The computational effort of this model is always very intensive on a uniform mesh. The adaptive hierarchical refinement approach[2] allows the three dimensional simulation to proceed efficiently. Three-dimensional numerical examples of domain evolution coupled to vesicle shape deformation are presented. Curvature-depended domain sorting and shape deformation dominated by line tension are also considered. REFERENCES [1] Embar, A., Dolbow, J.E. and Fried, E. “Microdomain evolution on giant unilamellar vesicles”, Biomech. Model. Mechanobiol, Vol. 12(3), pp. 597–615, (2013). [2] Jiang, W. and Dolbow, J.E., “Adaptive refinement of hierarchical B-spline finite elements with an efficient data transfer algorithm”, Int. J. Numer. Meth. Engng., doi: 10.1002/nme.4718 (2014).

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Multi-Scale Investigation of Failure Process in Brittle Polycrystalline Materials at High-Strain Rates

Author(s): Hao Jiang, Zongyue Fan, Bo Li, *Case Western Reserve U.*.

A novel multi-scale numerical model is presented to analyze the inelastic response and failure process in brittle polycrystalline materials subjected to dynamic loading. It is well recognized that the modes of fracture in competition and macroscopic dynamic strength of brittle materials are dependent on the microstructure features, including grain size and morphology, grain boundary, distribution of defects such as vacancies, second phase chemistry and stacking faults. The objective of the present work is to perform three dimensional numerical studies systematically and parametrically for a better understanding of the competition between intergranular and transgranular fracture as well as the interactions between crack and microstructure in brittle polycrystalline materials. In our simulations, the realistic 3D polycrystalline microstructures are reconstructed by incorporating experimental characterization data with stochastic and deterministic distributions of interfacial properties, grain morphology and crystallographic orientations. Quasi-continuum (QC) method is employed to integrate full atomistic calculations of the grain boundary with direct mesoscale simulations of grains. Intergranular fracture and the effect of defects resting at the grain boundaries on the crack path is studied via atomistic simulations. Transgranular fracture is simulated by the EigenFracture algorithm in the direct numerical simulation of the polycrystalline structure. The QC method is extended using the Optimal Transportation Meshfree (OTM) framework for a robust and efficient solution of dynamic behavior of materials at high strain rates involving extremely large deformations, fragmentation and comminution as well as dynamic contact.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: An Eulerian Method for Computation Shock Wave Problem with Meshfree RKPM Shock-Capturing and Non-Oscillation Schemes

Author(s): Jia-Hong Jiang , Chien-Ting Sun, Pai-Chen Guan, *Nat'l. Taiwan Ocean U.*.

Underwater explosion is usually simplified as the detonation of point explosives. In the beginning stage of the explosion, most of the released energy are converted into high-pressure and high-temperature gas bubbles in very short time (1, 2). During the procedure of bubble expansion, it generates the three-dimensional shock wave (discontinuous wave) propagation problem. Therefore, to properly simulate the phenomenon of shock waves in the water, the numerical methods must have a correct approximation of the discontinuity, a stable time integration method and the function to track the location of discontinuity. In this paper, we develop a non-oscillating reproducing kernel particle method (RKPM) for fluid dynamics problems for shock wave problems. To track the motion of shock front propagation, we introduce the indicator that automatic tracking the discontinuity location, using the first order derivative (slope) and second order derivative (curvature) to find the location of shock wave. The domain is then separated into shock front, regular and high order region with different requirement of shape functions. For different regions, we use the different RK shape functions to properly describe the shock, rarefaction and contact wave, and conform to total variable diminishing (TVD) method. The proposed method is tested by one-dimensional shock tube problem, the two-dimensional cavity flow and shock wave problems with bubble expansion. The results are compared with solutions and experiments. The proposed method shows the oscillation at the shock front is suppressed without artificial viscosity and any damping force. 1. Miller, S.T., Jasak, H., Boger, D.A., Paterson, E.G., Nedungadi, A., “A pressure-based, compressible, two-phase flow finite volume method for underwater explosions,” Computers & Fluids, Volume 87, 25 October 2013, Pages 132–143 2. Cole, R.H., “Underwater explosions,” Princeton University Press Press; 1948 Keywords: Non-Oscillating, Shock wave, Meshfree, RKPM, Fluid Dynamic

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Numerical Simulation of Fibrous Biomaterial with Randomly Distributed Fiber Network

Author(s): Tao Jin, Ilinca Stanciulescu, *Rice U.*.

Understanding the connection between the microscopic structure of fibrous biomaterials and their functionality is an important topic in tissue engineering. Many fibrous biomaterials have randomly distributed fiber network structures in the microscopic scale, and can be categorized as fiber-reinforced materials [1]. These fiber networks can undergo large deformations and exhibit significantly nonlinear behavior. The topology and the randomness of the fiber network at the microscopic level can largely influence the mechanical behavior of the material at the macroscopic level, for example, making the material isotropic, transversely isotropic or anisotropic [2]. This talk focuses on studying the influence of randomly distributed fiber networks on the mechanical behavior of fibrous biomaterials via numerical methods, specifically, using finite element analysis. In the first step, a 2D randomly distributed fiber network is generated with a random walk algorithm [3], with the fiber volume ratio and the length of individual fiber segments as controlling parameters. Then, the generated fiber network is embedded into a finite element mesh, and a special data structure is proposed to record the topological information of the network. The effects of large deformations and material nonlinearity are both considered. Since the aforementioned fiber network is randomly generated, the Monte Carlo (MC) method is used to simulate the material behavior in an average sense. Several numerical examples are provided to show that the computational framework used can not only incorporate the random fiber network structure into the finite element simulation without significantly increasing the computational cost, but can also capture the material nonlinearity and anisotropy. At last, the limitations of the methods used here and the future work are briefly discussed. Selected References: [1] D’Amore, A. et al., Biomaterials, Vol. 31, No. 20, 2010 [2] Nemir, S. et al., Biotech Bioeng, Vol. 105, No. 3, 2009. [3] Carleton, J.B. et al., Acta Biomaterialia, Vol. 12, 2015.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Nitsche Cut Finite Element Methods with Higher Order Elements

Author(s): August Johansson, *Simula Rsch. Lab.*; Mats Larson, *Umea U.*; Anders Logg, *Chalmers U. Tech.*.

We will present recent work on high order finite element methods for cut and composite meshes. The common theme is to use Nitsche's method to enforce conditions on boundaries or interfaces. The instabilities that may occur can be resolved in various ways. For a discontinuous Galerkin method it is possible to do a simple mesh-based element-wise association. Generally it is possible to add suitable stabilizing terms to the variational form. In this talk we will present Nitsche's method and two consistent alternatives for stabilizing a DG method and a CG method. We will show both theoretically and numerically that the proposed methods are optimal with respect to various norms.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A High-Order Discontinuous Galerkin Approach for Hydro Simulations of Strong Shocks and Material Interfaces

Author(s): Eric Johnsen, Marc Henry de Frahan, Mauro Rodriguez, *U. Michigan*.

We present a high-order accurate method for numerical simulations of strong shocks and material interfaces. Our focus lies in hydrodynamic instabilities between fluids of different density, such as Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz, driven by pressure/accelerations/velocities relevant to high-energy-density physics. Our numerical method is a high-order accurate Eulerian interface- and shock-capturing approach based on the high-order discontinuous Galerkin method. For this purpose, additional transport equations are solved in an appropriate form following the five-equations model, in addition to the balance of mass, momentum and energy equations, and a modified limiting procedure is used to regularize the solution. The high-order accuracy of the method improves the resolution of small-scale vortical flow features produced during these phenomena. We further discuss how such a procedure can be extended to include physical diffusion (of mass, momentum and energy) as well as viscoelasticity. We demonstrate the robustness of the proposed approach using multifluid and multiphase problems with strong shocks and large density ratios.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Mitigation of Zero-Energy Modes in Co-located Particle Methods

Author(s): Stephen Beissel, Gordon Johnson, *Southwest Rsch. Inst.*.

The development of meshfree and particle methods is often undertaken in the context of the weak form of the equations of motion. The methods must therefore incorporate a numerical integration scheme for evaluating the internal-work term of the equations. In the finite element method, subdivision of the spatial domain into elements provides guidance in the selection of an integration scheme, since each element contains shape functions of the same order. In contrast, and by design, particle methods lack a repeating subdivision of the domain and the corresponding order of the shape functions. While this lack of structure is advantageous for accommodating large deformations, it also obfuscates the optimal spatial integration scheme for a general distribution of nodes. Among the various integration schemes that appear in the literature, integration by sampling at the nodes (i.e., co-location of nodes and integration points) provides the simplest link between the order of the shape functions and the resolution of the integration scheme. This link is particularly important in computations involving large deformations because the nodal configurations change as the solution progresses. However, co-located particle methods have been known for years to suffer from zero-energy modes, e.g. [1]. This shortcoming appears to be inherent to co-location, since the zero-energy modes can be eliminated by moving the integration points to locations between the nodes. Chen and co-workers [2] have introduced a node-based integration scheme with stabilization of the zero-energy modes. This presentation examines several other methods for mitigating the zero-energy modes that accompany co-located particle methods, with the goal of improving the accuracy of large-deformation analyses. Spatial discretization is provided by the well established moving-least-squares method, avoiding the errors due to lack of linear completeness that plague the SPH method. The introduction of zero-energy modes is demonstrated by moving the integration points to the nodes. The methods for mitigating the zero-energy modes are compared. They include the bond viscosity that was developed for the SPH method, and integration schemes that incorporate the location of the nodes and derivatives of the integrands. [1] S. Beissel and T. Belytschko, “Nodal integration of the element-free Galerkin method,” Computer Methods in Applied Mechanics and Engineering 139 (1996), 49-74. [2] J. S. Chen, C. T. Wu, S. Yoon and Y. You, “A stabilized conforming nodal integration for Galerkin meshfree methods,” International Journal for Numerical Methods in Engineering 50 (2001), 435-66.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Smart Use of Density Functional Theory Calculations to Drive Newtonian Dynamics

Author(s): Reese Jones Jones, Michael Shaughnessy, *Sandia Nat'l. Lab.*.

We present a method for adaptively creating and sampling a database of density functional calculations in order to simulate large, complex atomistic systems at finite temperatures. The database consists of configurational/cluster-to-force maps and has a metric property via the Kabsch algorithm which we exploit in structuring the database for efficiency and accuracy. Details of the formulation including the correlation between local configuration size and force accuracy, will be discussed, as well as a number of practical applications of the method.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Extracting Coarse-Grained Dynamics of Extension Twinning in Magnesium Using Molecular Dynamics Simulations

Author(s): Shailendra Joshi, *Nat'l. U. Singapore*.

Magnesium (Mg) is a potential candidate for structural applications ranging from fuel-intensive automotive sector to biomedical components due to attractive properties such as low mass density, high damping capacity and excellent biocompatibility. There has been a renewed emphasis toward developing novel Mg microstructures with enhanced mechanical characteristics. It is imperative to understand the interactions between myriad deformation mechanisms in Mg to enable optimal microstructural design. Extension twinning is a ubiquitous mode of plasticity in this low-symmetry crystalline material. In this talk, we present a coarse-grained micromechanics landscape of extension twinning in single crystal Mg gleaned from molecular dynamics (MD) simulations. In particular, we extract the evolutions of overall twin volume fraction (v.f.), variant twin v.f. and twin number densities as a function of overall plastic strain extracted from this analysis provide a basis to construct constitutive laws for twin v.f. evolution in terms of nucleation, growth and coalescence. In doing so, we also investigate the effects of the inter-atomic potential, initial perturbations and loading rate. We discuss these results in the context of continuum crystal plasticity.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Thermomechanical Properties and Equation of State of \Gamma-RDX

Author(s): Kartik Josyula, Rahul ., Suvranu De, *RPI*.

In order to simulate the detonation pathways of an energetic material in continuum models, it is important to know the constitutive relations and the sensitivity of the model to pressure and temperature. The \gamma-polymorph plays an important role in the detonation mechanism of RDX. In our present work, we predict the thermomechanical properties of \gamma-RDX and their variation with pressure (4-11GPa) and temperature (200-550K) using a non-reactive fully flexible Smith and Bharadwaj (SB) molecular potential using molecular dynamics simulations (LAMMPS) [1]. The simulation cell is modeled after experimentally obtained crystal structure definition of \gamma-RDX [2] with non-orthogonal periodic boundary conditions. After equilibrating the system at 5.2GPa and 300K using isothermal-isostress ensemble, the pVT data is collected for calculating equation of state by equilibrating the system from 4-11GPa in increments of 1GPa and 200-550K in increments of 100K. At each equilibration point, a strain is applied on the system up to 10% in increments of 1% without straining the molecules internally and equilibrated using isothermal-isochoric ensemble at each increment. Then, the stress-strain data is used to calculate the elastic modulus tensor. The lattice parameters and unit cell volume of \gamma-RDX predicted by the simulation are consistent with experimental [2] and other simulation results [3]. The elastic modulus tensor calculated at 5.2GPa and 300K compares well with previous simulation data [3]. It indicates linear hardening and mild softening with pressure and temperature, respectively. This is consistent with similar observations of the \alpha-polymorph of RDX. A third order Birch Murnaghan equation of state has been proposed for \gamma-RDX which agrees well with previous simulation results. However, it over predicts the volume when compared with experimental data [2]. The coefficients of thermal expansion of \gamma-RDX are small in comparison to \alpha-RDX and show negligible variation with pressure and temperature. In particular, the b-lattice parameter is approximately constant with temperature, especially at high pressures. The present study provides invaluable information for modeling constitutive relations in continuum simulations for RDX, especially during shock loads. The absence of experimental material data on \gamma-RDX makes it even more significant. The stable and consistent results obtained using the SB potential, indicate the appropriateness of the potential in studying other molecular phenomena of RDX. References: 1. Josyula et al., RSC Adv. 4, 41491 (2014). 2. Davidson et al., CrystEngComm 10, 162 (2008). 3. Munday et al., J. Phys. Chem. B 115, 4378 (2011).

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Hausdorff Dimension Estimation via Elastodynamic Excitation of Fractal Media

Author(s): Hady Joumaa, *RHU*.

Fractal media, whether of geometric or natural type, are characterized by their highly irregular topology which cannot be conceived by the well-known elements of Euclidean geometry [1]. The Hausdorff dimension, D, which essentially estimates the degree of deviation from smooth-like topology, is, as discovered in previous research work, an influential factor in prescribing the elastodynamics of fractal bodies. In measure theory, D is defined through the self-similarity property of fractal sets and it can be evaluated exactly for geometric fractals [1,2]. For some natural fractals, D is the exponent in the power law equation which defines the mass of the involved natural fractal. Also, for some fractal sets, D can be estimated through statistical methods (e.g. box counting method, sausage method,...)[1,2]. Nevertheless, to accurately perform the estimation of D, these methods necessitate the acquisition of high-precision images which is often cumbersome to realize, particularly when the fractal body is of anisotropic type, i.e. D is not uniform but direction dependent. As a result, a novel technique in which these various imposed difficulties are overcome without undermining the mathematical and physical robustness of the previously discussed statistical methods, is crucial to achieve the estimation of the Hausdorff dimension. The objective of this research is to present and discuss a technique whereby the Hausdorff dimension of a fractal body is estimated through its elastodynamic excitation, thanks to the significant advancement achieved in the topic of elastodynamics in fractal media. In the past few years, the elastodynamics of fractal bodies has been intensively studied, and different continuous-like fractal models have been established, thus incorporating the fundamental conservation laws of mechanics into the framework of the so called "fractal mechanics". In particular, the phenomena of wave propagation due to free vibration for both isotropic and anisotropic fractal media has been analysed [3]. Various problems involving modal decomposition were simulated through both analytical and computational means. In these simulations, valuable findings were discovered whereby the effect of D on the natural frequencies, w_n, is highlighted. The correlation between D and w_n constitutes the core concept on which the method to estimate D is founded. Once the fractal body is excited, the time response is then transferred to the frequency domain through Fourier transform and consequently, the body's inherent frequency spectrum is revealed, and D is finally estimated. The significance of this technique lies in the feasibility of its experimental realization. The involved specimen testing is of standardized type and so is the subsequent data analysis. In our work, we have performed various elastodynamic simulations for both isotropic and anisotropic fractal bodies aiming to confirm the accuracy of this introduced technique. References: [1] - Falconer, K.: Fractal Geometry: Mathematical Foundations and Applications. Wiley, England (2003) [2] - Hastings, H.M., Sugihara, G.: Fractals: A User’s Guide for the Natural Sciences. Oxford Science Publications, Oxford (1993) [3] - M. Ostoja-Starzewski, J. Li, H. Joumaa, and P.N. Demmie: From fractal media to continuum mechanics, invited review, Zeit. Angew. Math. Mech. (ZAMM) 93, 1-29, 2013.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Shape and Topology Optimization via the Level Set Method

Author(s): François Jouve, *Paris Diderot U.*.

Shape and topology optimization via the level set method has started attracting the interest of an increasing number of researchers and industrial designers over the past years. A large number of academic problems, using various objective functions and constraints, have been successfully treated with this class of methods, showing its efficiency and flexibility. But real industrial applications may involve more complex and mixed constraints than classical optimal design problems. Moreover, they are sometimes not easy to formulate from a mathematical point of view, and even more difficult to handle numerically. Examples of such real life problems will be shown at the conference.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Mixing in Particulate Flows: 2D Vesicle Suspensions

Author(s): Gokberk Kabacaoglu, George Biros, Bryan Quaife, *UT Austin*.

Particulate flows are ubiquitous in various applications such as biological flows. Here we study mixing in vesicle suspensions. Vesicles are deformable capsules that resist bending and are locally inextensible. They are experimental and numerical proxies for red blood cells and other biological capsules. This study aims to extend our group's work on the simulation of two-dimensional vesicles suspended in a Stokesian fluid [1] by investigating mass transport from vesicles and hence mixing in their environment. In order to understand the physics of mixing, we focus on the flow in a Couette apparatus where the mass transport is modeled with an advection-diffusion equation and is solved numerically with a collocation method. The geometry is discretized with high-order accuracy by using a Fourier representation for the azimuthal direction and a Chebyshev representation for the radial direction. The time integration is done with first and second order implicit-explicit (IMEX) schemes [2]. Finally, the mass transport equation is coupled with the vesicle suspension through the velocity field and the initial condition. In advection-dominated flows (i.e. high Peclet number flows), mixing is highly dependent on perturbations in the velocity field due to the presence of vesicles and flow boundaries.. Therefore, it is necessary to capture these perturbations by running the vesicle simulations so that they are reflected to the mass transport problem. Additionally, there is no broad agreement on what constitutes a good measure of mixing quality. In this study, we use the so-called Mix-Norm defined by a Sobolev norm of negative index [3]. We study the transport of various species in the cases of different viscosity contrasts between the vesicle and the flow, and shear rates. Consequently, quantifying mixing in these cases and comparing them with no-vesicle results deliver a limiting Peclet number at which the incorporation of the vesicle simulation is rendered essential. [1] B. Quaife, G. Biros, Journal of Computational Physics, 274: 245-267, 2014. [2] U. M. Ascher, S. J. Ruuth, B. Wetton, SIAM J. Numer. Anal., 32: 797-823, 1995 [3] G. Mathew, I. Mezic, L. Petzold, Physica D-Nonlinear Phenomena, 211: 23-46, 2005.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling of Lamellar Fracture of Polysynthetically Twinned (PST)-TiAl Crystals Using Cohesive Zone Models and XFEM in a Two-Scale FE Approach

Author(s): Mohammad Rizviul Kabir, Marion Bartsch, *German Aerospace Center (DLR e.V)*.

The mechanical behavior of intermetallic TiAl alloys is influenced by the morphology of single phase (gTiAl) grains and two-phase (a2Ti3Al+gTiAl) lamellar structures. To understand the role of the lamellar structures for the deformation and fracture behavior of TiAl alloys, a crystal plasticity based FE model (CPFEM) has been developed that takes important microstructural information and anisotropic phase properties into account and considers local fracture behavior within the lamellar phases. The lamellar microstructure consists of relatively thin a2Ti3Al and thick gTiAl plates. Between two a2Ti3Al plates many gTiAl lamellae are located. For modeling purpose the lamellar microstructure has been described in a FE unit cell using representative volume elements (RVE) based on an ideal description of the lamellar phases with the average vol.% of the phases and their respective orientations. Two types of lamellar fracture have been described in this unit cell. One is the interlamellar fracture that occurs due to interface failure at the g/g or a2/g interfaces, and the other is the translamellar fracture that occurs due to cleavage of the bulk gTiAl phases. For the numerical description of interlamellar fracture the phase boundaries are designed with cohesive interfaces to capture debonding damage. On the other hand, the translamellar fracture has been modeled using an XFEM approach combined with cohesive damage behavior which allows one to model material splitting due to cleavage. This unit cell has been embedded in a macro-scale FE model for describing overall response of the lamellar structure. First order homogenization approach is used to couple these two models. For the macroscopic damage behavior a modified homogenization approach for cohesive damage has been assumed where the discrete crack has been modeled in the unit cell and in macro FE elements. The micromechanical deformation of the phases has been described using a classical CPFEM model. The model parameters for the crystal plasticity have been estimated fitting the stress-strain response obtained from tensile experiments on lamellar polysynthetically twinned (PST)-TiAl crystals. The cohesive model parameters are estimated by adjusting the numerical fracture behavior with the experimental fracture response for this PST-TiAl alloy. In this presentation we will demonstrate the models ability to predict interlamellar and translamellar fracture of PST crystals under different lamellar orientation condition. Furthermore, macroscopic failure will be predicted based on the unit cell calculations.

13th U.S. National Congress on Computational Mechanics
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Title: A Critical Comparison of C1-Continuous Methods Applied to the Cahn-Hilliard Equation

Author(s): Stefan Kaessmair, Paul Steinmann, *U. Erlangen–Nuremberg*.

Diffusive phase separation may describe various phenomena that are observed in nature, such as tumor-growth, mineral unmixing, or the formation of microstructures in alloys. In order to adequately model these processes, Cahn and Hilliard propose a free energy function composed of a non-convex configurational part and a contribution accounting for the interface energy. In a two stage process, the mixture first decomposes into the so called pure phases associated with the local minima of the configurational free energy, followed by coarsening the pattern of the pure phases to minimize the interface energy. The fourth-order Cahn–Hilliard equation necessitates piecewise smooth and globally C1-continuous basis functions or the application of mixed methods based on a second-order split. The latter provides an elegant way to solve the Cahn–Hilliard equation but requires the introduction of an new variable in addition to the primal unknown. Thus, C1-continuous methods are of particular interest, since they only incorporate the primal unknown. In the present contribution, the isogeometric analysis, using a C1-continuous spline basis, and the natural element method based on the Farin interpolant, are considered in a two- and three-dimensional case. It has been shown in [1] and in [2], respectively, that the isogeometric analysis as well as the natural element method are capable of solving the Cahn–Hilliard equation. Nevertheless, a comparison of both methods reveals the individual strengths and weaknesses of both methods. The second order splitting method described in [3] serves as a reference to which both higher order methods are compared. Acknowledgements The support by the German Research Foundation (DFG) under grant STE 544/48-1 is gratefully acknowledged. References [1] H. Gómez, V.M. Calo, Y. Bazilevs, T.J.R. Hughes. Isogeometric analysis of the Cahn–Hilliard phase-field model, Comput. Methods Appl. Mech. Engrg. 197 (2008), 4333–4352. [2] A. Rajagopal, P. Fischer, E. Kuhl, P. Steinmann. Natural element analysis of the Cahn-Hilliard phase-field model. Computational Mechanics 46 (2010), 471–493. [3] R.L.J.M. Ubachs, P.J.G. Schreurs, M.G.D. Geers. A nonlocal diffuse interface model for microstructure evolution of tin-lead solder, Journal of the Mechanics and Physics of Solids 52 (2004), 1763–1792.

13th U.S. National Congress on Computational Mechanics
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Title: Coupling of Multi-Resolution Continuum Theory and Dislocation Dynamics for Physically Informed Component Scale Simulation

Author(s): Orion L. Kafka, Jacob Smith, John A. Moore, Miguel Bessa, Wing Kam Liu, *Northwestern U.*; Tarek Hatem, *British U. Egypt*.

Advancing the safety and efficiency of materials and designs requires development of techniques to tractably include detailed material simulation within component and system scale models. To this end, we combine a formulation of Multiresolution Continuum Theory (MCT) within the finite element method with a dislocation dynamics material model derived as an extension from the Orowan creep strain equation. The purpose here is to capture the plastic strain evolution efficiently, and with a sound physical basis at the micro-scale, while conducting component-scale simulations. In the macro-scale MCT law, we employ a J2 metal plasticity model where the hardening law for the matrix flow stress is governed by the solution of the Orowan equation and thus by the associated differential equations that describe mobile, static, and boundary dislocation densities. Additionally, in implementation of this scheme, the MCT length-scale is a parameter derived from crystal plasticity calculations, supplying further physical meaning to the MCT model. MCT allows for more sophisticated localization modeling than pure dislocation dynamics models. Our method is computationally inexpensive, particularly when compared to crystal plasticity calculations. This algorithm was implemented in the finite element analysis package LS-DYNA, using both a user element subroutine to implement MCT and a user material to perform the calculations required by the material model. This procedure is applied to simple test cases for comparison with experimental results and prior simulations. Possible extensions to this model include the addition of material laws at different scales within MCT and further development of the failure surface calculations currently employed.

13th U.S. National Congress on Computational Mechanics
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Title: Structure, Properties and Function of the Human Femoropopliteal Artery

Author(s): Alexey Kamenskiy, Jason MacTaggart, *U. Nebraska Med'l. Center*.

Peripheral artery disease (PAD) frequently refers to atherosclerotic obstruction of the femoropopliteal artery (FPA) reducing blood flow to the lower limb. Reconstructive therapies for PAD are notorious for high failure rates, and understanding of the FPA's structure and properties could better elucidate its function and improve models of the artery and repair techniques, materials and devices. Fresh FPAs were obtained from n=190 human subjects, age 13-80 years old. In situ vs excised arterial lengths, and circumferential and longitudinal opening angles were measured for all arteries. Transverse and longitudinal arterial segments were analyzed with Verhoeff-Van Gieson staining, and data on arterial structure were used to define the strain energy function incorporating the passive contributions of ground substance, elastin, collagen, and smooth muscle. Mechanical property characterization was performed using quasi-static multi-ratio planar biaxial extension, and physiologic stress-strain state was determined by constitutive modeling. Histopathological analysis demonstrated that FPA wall structure supports its function as a muscular artery in the severe mechanical environment of the flexing limb. The majority of the FPA wall thickness is comprised of smooth muscle cells that regulate arterial diameter in response to downstream flow demands. Elastic recoil after locomotion-induced deformation is facilitated by elastin fibers that are mainly concentrated in the External Elastic Lamina (EEL). These fibers are oriented longitudinally in parallel laminae and are under significant tension in healthy young FPAs. This residual tension of the EEL is largely responsible for the in situ longitudinal pre-stretch which reduces kinking of the artery during limb flexion and ensures energy efficient function by decoupling internal pressure and tethering force. The EEL also likely plays a major role in FPA adaptation. As the artery stiffens with aging and disease, the fibers of the EEL degrade and fragment, reducing the physiological longitudinal stress to maintain stable circumferential stress. These adaptations, influenced by classic clinical risk factors such as hypertension, diabetes and coronary artery disease, are reflected histopathologically by attenuated and fragmented elastin fibers and thinner EEL which in turn result in decreased in situ pre-stretch, more kinking of the FPA during locomotion and loss of energy efficient function. Detailed understanding of the FPA structure, properties and function in the context of the mechanical and biological environments, can improve our understanding of PAD pathophysiology and guide development of better treatment methods and devices through more realistic computational modeling and simulation.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Immersogeometric Fluid–Thin Structure Interaction Analysis: Enhanced Conservation and Application to Heart Valve Simulation

Author(s): David Kamensky, Michael S. Sacks, Thomas J. R. Hughes, *UT Austin*; Ming-Chen Hsu, *Iowa State U.*; John A. Evans, *U. Colorado-Boulder*.

In this work, we develop a framework for computational simulation of fluid–structure interaction (FSI) that employs a spline-based representation of the structure geometry and an unfitted mesh of the surrounding fluid domain. The variational fluid and structure subproblems are coupled weakly through an augmented Lagrangian. Our framework fits into the paradigm of immersogeometric analysis: it captures the geometry of a partial differential equation's domain on an unfitted analysis mesh. We apply this framework to simulation of a bioprosthetic heart valve (BHV). To analyze BHVs, we are specifically concerned with the limit of thin immersed structures. The structural mechanics are modeled using Kirchhoff–Love shell theory and discretized isogeometrically in space. The thin structure geometry is modeled as a surface of co-dimension one to the fluid domain. The exact fluid solution has pressure discontinuities and sharp velocity features along the immersed surface. This implies that the distance between the exact fluid solution and the discrete solution space of the unfitted background mesh will converge sub-optimally with refinement. In practice, the effect of this local interpolation error on the solution away from the immersed structure depends critically on the conservation properties of the numerical method, and we must take special measures to improve conservation. These measures include a new semi-implicit time integration scheme for the Lagrange multiplier field, modifications to stabilized fluid formulations, and divergence-conforming fluid discretizations. We demonstrate the effectiveness of the numerical method by comparing its results with boundary-fitted reference solutions to benchmark problems. To investigate the validity of our BHV modeling, we compare FSI computations with flow loop experiments that measured the deformations of BHV leaflets in vitro.

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Title: A Local XFEM Method for the Simulation of Multi-Fluid Flows Using the Particle Level Set Method

Author(s): Kazem Kamran, Riccardo Rossi, Eugenio Oñate, *CIMNE - UPC*.

The simulation of immiscible two-phase flows on Eulerian meshes requires the use of special techniques to guarantee a sharp definition of the evolving fluid interface. This work describes the combination of two distinct technologies with the goal of improving the accuracy of the target simulations. First of all, a spatial enrichment1 is employed to improve the approximation properties of the Eulerian mesh. This is done by injecting into the solution space new features to make it able to correctly resolve the solution in the vicinity of the moving interface. Then, the Lagrangian Particle Level Set (PLS) method2 is employed to keep trace of the evolving solution and to improve the mass conservation properties of the resulting method. While the local enrichment can be understood in the general context of the XFEM, we employ an element-local variant, which allows preserving the matrix graph, and hence highly improving the computational efficiency. Basically, at each cut element the pressure field is enriched at the element level and then condensed prior to the assembly. Although no enrichment for the velocity field is considered, numerical results show that the method perfectly works for the physical problems dominated by gravitational forces. Numerical results suggest that, at least for tetrahedral meshes, the inclusion of PLS to overcome the mass gain/loss is crucial in examples undergoing large deformations of the interface. Our results compare well with those obtained with standard XFEM using hexahedral meshes. And in some cases are superior in determining the interface evolution. REFERENCES [1] Henning Sauerland and Thomas-Peter Fries, “The extended finite element method for two-phase and free-surface flows: A systematic study”, Journal of Computational Physics, 230(9):3369-3390 (2011). [2] Douglas Enright, Ronald Fedkiw, Joel Ferziger, and Ian Mitchell, “A hybrid particle level set method for improved interface capturing”, Journal of Computational Physics, 183(1), 83-116 (2002).

13th U.S. National Congress on Computational Mechanics
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Title: Fluid-Structure Interaction Analysis of a Disk-Gap-Band Parachute in Compressible-Flow Regime

Author(s): Taro Kanai, Kenji Takizawa, *Waseda U.*; Tayfun Tezduyar, *Rice U.*.

The Mars exploration systems, which are currently being developed both by NASA and Japan Aerospace Exploration Agency (JAXA), will require parachutes to decelerate the capsule from supersonic to subsonic speeds after entering the Mars's atmosphere. A disk-gap-band (DGB) parachute will be deployed for this purpose. This parachute has a design that originates from those used with earlier spacecraft such as Viking. An important consideration is Mars's atmospheric composition, which has a density that is one-hundredth of that of the Earth's atmosphere. This, and the issues related to scaling down the parachute structure, make wind tunnel test under actual flight conditions basically impossible. This creates a clear and rather crucial role for computational analysis, which can of course be performed under actual flight conditions. With a core computational technology and a set of special techniques targeting parachutes, we intend to bring reliable solution and analysis to this class of problems. Our analysis will take into account the fluid-structure interaction (FSI) between the DGB parachute and the compressible flow the parachute is subjected to. To increase our confidence in the solution techniques we use, we plan to first focus on the analysis under wind tunnel conditions, so that we can compare our results to some physical data. Once we feel comfortable with the results, we plan to move to the cases under actual flight conditions. We plan to use NURBS basis functions to represent the geometry, which will give us a smoother representation than a typical finite element approximation. The structural and fluid mechanics formulations will also be based on using NURBS basis functions. Our eventual target in this analysis is to help improve the parachute design by having a good balance between reducing the average speed and reducing the speed fluctuations.

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Title: A Finite Element-Based PML Method for Time-Domain Electromagnetic Wave Propagation Analysis

Author(s): Sangri Yi, Namho Joh, Boyoung Kim, Jun Won Kang, *Seoul Nat'l. U.*.

This study is concerned with the development of new mixed unsplit-field perfectly-matched-layers (PMLs) for the simulation of plane electromagnetic waves in heterogeneous unbounded domains. The development of the electromagnetic PML targets the application to engineering mechanics problems such as structural health monitoring and inverse medium problems. To formulate the unsplit-field PML, a complex coordinate transformation is introduced to Maxwell's equations in the frequency-domain. The transformed equations are converted back to the time-domain by the inverse Fourier transform to arrive at governing equations for transient electromagnetic waves within the PML-truncated computational domain. Upon spatial discretization based on a mixed finite element method, the resulting equations lead to a mixed semi-discrete form, where both electric and magnetic fields are treated as independent unknowns. A special pair of basis functions for the approximation of electric and magnetic fields is introduced for the stability of numerical solutions. The developed PML method is computationally straightforward when compared to split-field PML techniques [1]. It also allows the use of relatively simple temporal schemes for integration of the semi-discrete form, by contrast to the PML methods requiring the calculation of complicated convolution integrals [2] or the use of finite difference methods. Numerical results are presented for plane microwaves propagating through concrete structures, and the accuracy of solutions is investigated by a series of error analyses. [1] F. Collino and C. Tsogka (2001). "Application of the perfectly matched absorbing layer model to the linear elastodynamic problem in anisotropic heterogeneous media." Geophysics, Vol. 66, No. 1, pp. 294-307. [2] R. Matzen (2011). "An efficient finite element time-domain formulation for the elastic second-order wave equation: A non-split complex frequency shifted convolutional PML." International Journal for Numerical Methods in Engineering, Vol. 88, No. 10, pp. 951-973.

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Title: Implicit Large-Eddy Simulations of Single and Counter-Rotating Vertical-Axis Wind Turbines in the Low-Reynolds Regime Using a High-Order DG Method

Author(s): Samuel Kanner, Per-Olof Persson, Luming Wang, *UC Berkeley*.

A high-order Implicit Large Eddy Simulation (ILES) method in 2D and 3D is used to simulate a section of a constant spinning straight-bladed vertical-axis wind turbine with two blades at low-Reynolds numbers (Re<10^5). The complex domain deformations for the counter-rotating case is handled by a combination of element topology flipping and local L^2 projections, which results in an efficient scheme with arbitrarily high order of accuracy and exact conservation. The magnitude of the blade forces are analyzed and compared to analytical codes and experiments. The maximum power coefficient was found at a tip-speed ratio of 5.0. The pitch angle of the blades are varied in order to take into account the uncertainties in the mounting angle of the blade in the experimental studies for the single turbine. As found previously, a small toe-out angle can increase the power absorption of the turbine by nearly 10%. Further, depending on the incident wind direction, a synergistic effect can occur for counter-rotating turbines. Over a range of tip-speed ratios, the computed tangential forces as a function of the azimuthal angle agree much better to the experimental data at high tip-speed ratios as compared to other, lower-fidelity analytical turbine codes. The wake structures and flow field are visualized to elucidate the mechanism behind the increased power production. In this study we aim to determine whether the increased power production for the counter-rotating case found empirically by Prof. Dabiri (Dabiri, J. Renewable and Sustainable Energy, 3, 043104, 2011), can be partly explained by the 2D flow field.

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Title: On Lattice Boltzmann Methods for Flow and Transport Problems in Porous Media

Author(s): Saeid Karimi, Kalyana Babu Nakshatrala, *U. Houston*.

Lattice Boltzmann methods are routinely used to simulate flow in porous media. Implementation of these methods in a parallel and heterogeneous computing setting is natural. One of the key advantages of the lattice Boltzmann methods over other conventional methods is its capability to handle complicated domain geometries. This feature is specifically useful in porous media simulations due to the irregular geometry of fractures and pores. Furthermore, because of the origins of this method in kinetic theory, incorporating results from kinetic theory into the simulation is much easier than it is in continuum-based methods. In recent years, numerous advances have broadened the range of application of lattice Boltzmann methods to advection-diffusion-reaction problems. Different reaction models, either linear or non-linear, can be included in the numerical solution with relative ease. In this presentation, we will give an overview of recent efforts in designing lattice Boltzmann methods for advection with anisotropic diffusion. Some key results regarding these methods will be presented. Several numerical examples will be used to examine the performance of these methods in the context of transport, and chemical reactions. Based on the findings, a guideline for future developments in this field will be suggested.

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Title: Non-Symmetric Coupling of Boundary Elements and Ultraweak Finite Elements and DPG Method with Optimal Test Functions

Author(s): Norbert Heuer, Michael Karkulik, *PUC Chile*.

We propose and analyze a numerical method to solve an elliptic transmission problem in full space. The method consists of a variational formulation involving standard boundary integral operators on the coupling interface and an ultraweak finite element formulation on the interior. To be precise, it is a nonsymmetric coupling as developed in [Johnson-Nédélec, Math. Comp., 1980], but with an ultraweak finite element part as used in [Demkowicz-Gopalakrishnan, SIAM J. Numer. Anal., 2011]. To guarantee the discrete inf-sup condition, we discretize the whole system with optimal test functions. In this way, we obtain quasi-optimality of the method in the so-called energy norm. In order to relate the energy norm to usual Sobolev norms, we use recent results regarding the nonsymmetric coupling of finite elements and boundary elements on polygonal interfaces, cf. [Sayas, SIAM Rev., 2013].

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Title: Phase-Field Modeling of Propagation and Coarsening of Segmented Crack Fronts in Mode I+III Fracture

Author(s): Alain Karma, Matteo Nicoli, *Northeastern U. Boston*; Veronique Lazarus, *U. Paris-SUD, CNRS*.

Quasistatic crack propagation in mixed mode I+III fracture is widely observed to be unstable. The instability is characterized by the segmentation of the parent crack into a periodic array of daughter cracks. The daughter cracks also known as fracture lances are shaped as flat facets rotated towards the principal stress axis. We report on progress to characterize this instability through a combination of three-dimensional phase-field simulations, theoretical calculations in the framework of linear elastic fracture mechanics, and in situ observations of the dynamical evolution of the crack front in PMMA three point bending experiments. The results show that the formation of fracture lances is strongly subcritical as a function of the ratio K3/K1 of the mode III and mode I stress intensity factors. They also demonstrate that the coarsening of facets in both simulations and experiments is characterized by a linear scaling relationship between the facet width and propagation length with a prefactor that is strongly dependent on K3/K1. An approximate analytical theory is developed to predict the dependence of the facet rotation angle on K3/K1, showing a good agreement with angles observed in both simulations and experiments.

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Title: dfnWorks: A Discrete Fracture Network Framework for Modeling Flow and Transport in Fractured Porous Medium

Author(s): Satish Karra, Jeffrey Hyman, Nataliia Makedonska, Hari Viswanathan, Carl Gable, *Los Alamos Nat'l. Lab.*; Scott Painter, *Oak Ridge Nat'l. Lab.*.

Several subsurface related applications including unconventional oil & gas, CO2 sequestration and storage, nuclear waster repository science, involve understanding flow and transport in fractured rock. Discrete fracture network (DFN) modeling provides a promising alternative to continuum-based approaches (such as stochastic continuum, dual/multiple continuum) for computational simulations of fluid flow and transport through sparsely fractured rocks in the subsurface. In this approach, fractures are explicitly represented as two-dimensional planes in three-dimensions where these planar fractures are stochastically generated based on geologic site information such as fracture orientation, shape, location and aperture distributions. Once these DFNs are generated, they are meshed and flow is solved on these meshes. The capability to include detailed site information leads to more accurate representation of the medium in contrast to using effective properties in continuum approaches. However, the DFN approach is well known to be computationally intensive and to overcome this drawback techniques are used to upscale average properties that feed into a continuum based approach. In this talk, details of a high performance computational suite dfnWorks that has been recently developed at the Los Alamos National Laboratory to overcome the drawbacks of the DFN approach, will be presented. This suite uses a state-of-the art feature rejection algorithm for stochastically generating DFNs, the LaGriT toolbox for mesh generation, the massively parallel code PFLOTRAN for solving flow and a recently developed algorithm for particle tracking on DFN to examine transport. Recent applications of this suite to subsurface problems along with new data analytics that have been only possible due to the HPC capability of the dfnWorks suite will also be discussed.

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Title: Modeling, Simulation and Visualization of Tsunami

Author(s): Kazuo Kashiyama, *Chuo U.*.

Tsunami kill many human beings and damages economic activities seriously, such as tsunami caused by the Great East Japan Earthquake in 2011. It is very important to develop a useful modelling and simulation methods for tsunami waves in order to perform the planning and design for the community development and the prevention of disaster. The visualization is also important to understand the power of tsunami and to improve the consciousness of disaster prevention. Recently, the visualization using the virtual reality (VR) and augmented reality (AR) technology is becoming more popular for the visualization of three dimensional numerical simulations. In this presentation, the modelling, simulation and visualization methods are presented for tsunami waves. The stabilized finite element methods are employed for 2D and 3D tsunami simulations using the shallow water equation, Boussinesq equation and Navier-Stokes equation. In order to realize an efficient numerical simulation, a combination method using 2D and 3D models is presented. We also propose a visualization system using virtual reality technology to improve the quality of education for disaster prevention. The present modelling, simulation and visualization methods are shown to be useful tools to realize the high quality computing for large scale tsunami simulation.

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Scale Topology Optimization For Hyperelastic Composites

Author(s): Junji Kato, *Tohoku U.*.

The present paper addresses topology optimization of both micro- and macro-structure for inelastic composite materials applying a decoupling multi-scale analysis. In structural mechanics, microscopic material behavior plays a significant role in controlling the entire structural response, especially on the materially and/or geometrically nonlinear regime. In the present study the end compliance of a macrostructure is maximized with respect to material volume fraction of composite at the microstructure together with material density at the macrostructure. In order to observe mechanical behavior of microstructure, we apply multi-scale analysis based on a homogenization method. The general multi-scale strategy considering material nonlinearity encounters to huge amounts of computations. In the meanwhile a new multi-scale strategy, so-called the decoupling multi-scale analysis [1] has been developed to reduce the computational costs. The present study applies this scheme for multi-scale topology optimization based on our previous study [2] and extends it to hyperelastic model. In this process, we propose a consistent analytical sensitivity utilizing a localization process. The performance of the proposed method is demonstrated by a series of numerical examples. Finally, it is verified that the proposed method has a great potential for material design assuming materially and/or geometrically nonlinear structural problems. References [1] K. Terada, J. Kato, N. Hirayama, M. Inugai, K. Yamamoto, A method of two-scale analysis with micro-macro decoupling scheme: application to hyperelastic composite materials, Computational Mechanics, 49, 595-608, 2014. [2] J. Kato, D. Yachi, K. Terada, T. Kyoya, Topology optimization of micro-structure for composites applying a decoupling multi-scale analysis, Structural and Multidisciplinary Optimization, 52, 1199-1219, 2013.

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Title: Performance Comparison of Subdomain Local Solvers in Domain Decomposition Method

Author(s): Hiroshi Kawai, *Tokyo U. Science-Suwa*; Masao Ogino, *Nagoya U.*; Ryuji Shioya, *Toyo U.*; Tomonori Yamada, Shinobu Yoshimura, *U. Tokyo*.

Domain Decomposition Method (DDM) is one of the promising parallel schemes for finite element analysis. Subdomain-level local solver plays an essential role in DDM in general, and especially in non-overlapping type iterative substructuring method, and it can easily be the performance bottleneck on modern supercomputing environments. Here in this presentation, the authors compare various kinds of implementation about DDM subdomain local solvers, such as direct and iterative solver-based, on several types of high performance computing environments and architectures.

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Title: Dislocation Dynamics Modeling of Slip-System Interactions in FCC Metals

Author(s): Haruka Kawate, Akiyuki Takahashi, *Tokyo U. Science*.

Strain hardening is a result of strong mutual interaction between slip-systems. Therefore, in order to understand quantitatively the strain hardening, it is necessary to consider the interaction between dislocations of different slip-systems. Up till now, there is an attempt to evaluate the strength of the interaction between two slip-systems using the dislocation dynamics method, and however, the results show a different trend from the corresponding experimental results. This must be attributed to the fact that the dislocation dynamics simulation deals with only two slip-systems, whereas, in the experiments, there are twelve slip-systems. In this study, the interaction between slip systems in a FCC metal is investigated using the 3-dimensional dislocation dynamics method as a numerical modeling of strain hardening behavior. First, the interaction between two slip-systems is simulated, and the flow stress increase due to the interaction is evaluated. The trend of the flow stress increase obtained in this study is very similar to that obtained by the past dislocation dynamics simulation studies. Next, we performed the dislocation dynamics simulation with twelve slip-systems. According to the experimental procedure, the crystal model is first subjected to a tension loading with a certain amount. Then, the tension loading is removed (unloading), and another tension loading in a different direction is given to the crystal model. Using the procedure, the dislocation density is increased in a slip system by the first tension loading, and the dislocation interaction can be taken place by the second tension loading. In the results, the trend of the flow stress increase is in good agreement with the experimental results. It must suggest that not only the primary slip-system, and also the secondary slip-system must be activated well in the experiments, and gives significant influence to the experimental results.

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Title: High-Order Shape Functions for Exact Sequence Elements of All Shapes: Part I Methodology

Author(s): Brendan Keith, Federico Feuntes, Leszek Demkowicz, *UT Austin*.

ESEAS [1] is a new high order shape function library which stands for Exact Sequence for Elements of All Shapes. It is a collection of hierarchical shape function routines written in Fortran for 1D, 2D, and 3D finite element software. Specifically, the library has routines for the segment in 1D, the triangle and quadrilateral in 2D, and the hexahedron, tetrahedron, prism, and pyramid in 3D. Together, we refer to these geometries as the elements of 'all shapes.' ESEAS computes all shape functions for all shapes with the unifying methodology of projecting, evaluating, and blending. The library treats each shape function in the same way, and across all elements and all energy spaces it relies upon only 8 coordinate-free 'ancillary functions' for the evaluation step. For each element, the shape functions in ESEAS are conforming to each Sobolev energy space of its corresponding exact sequence. In particular, for each element, the shape functions in ESEAS conform hierarchically in p, to H1, H(curl), H(div) and L2, when defined. When applicable, the discrete energy spaces correspond to the well-known Nédélec spaces, and are suitable for hybrid meshes. For some of the well-studied elements, the shape functions agree with those existing in the literature which have been optimized for sparsity. Some additional features of ESEAS are that it easily facilitates fast integration and orientation embeddings. In this talk, I will present the methodology used in writing ESEAS and give some examples for standard 2D and 3D elements. Part II will focus on applications to the Pyramid element. A report expanding upon this methodology and detailing the construction of each shape function is available in [2]. Simple visual examples of these shape functions for 2D elements will be presented here along with further details of the aforementioned features of ESEAS. [1] ESEAS library: https://github.com/libESEAS/ESEAS [2] Fuentes, F., Keith, B., Nagaraj, S., Demkowicz, L. (2015). High Order Orientation Embedded Finite Element (FE) Shape Functions for the Exact Sequence Elements of All Shapes. ICES Reports, UT Austin.

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Title: A Crystal Plasticity Temperature and Orientation Dependent Constitutive Model in Nickel-Based Superalloys

Author(s): Shahriyar Keshavarz, *Nat'l. Inst. Standards & Tech.*; Somnath Ghosh, *Johns Hopkins U.*.

A dislocation density-based non-Schmid constitutive model is developed to address the asymmetry in tension and compression as well as orientation dependent of the single crystal of Nickel-based superalloys for a wide temperature range. The size-dependent, dislocation density-based FEM model of the sub-grain scale representative volume element (RVE) with explicit depiction of the morphology is employed for simulation in the crystal plasticity framework. Consistent with observations made for a wide temperature range from room temperature to 1000oC, mechanism of anti-phase boundary (APB) is considered in the model. The non-Schmid constitutive model incorporates hardening evolution due to Statistically Stored Dislocations (SSDs), Geometrically Necessary Dislocations (GNDs) and cross-slip dislocations (CSDs). Experimental data for Ni-base single crystals, available in the literature, are used to calibrate material parameters. Subsequently results of crystal plasticity FEM simulations are compared with experimental data for several orientations in constant strain-rate and creep tests at a wide range of temperatures. The model is able to correctly predict the response of Ni-base single crystals including tension and compression asymmetry.

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Title: A Gradient Based Approach for Reliability Based Design Optimization via Stochastic Expansion Methods

Author(s): Vahid Keshavarzzadeh, Daniel Tortorelli, *U. Illinois, Urbana-Champaign*.

We present a gradient based approach for reliability based design optimization employing stochastic expansion methods. An accurate and efficient uncertainty propagation scheme based on polynomial chaos expansion is used to evaluate the probabilities of the cost and constraint functions [1,2]. Both intrusive and non-intrusive polynomial chaos approaches are employed in the design optimization process. The statistical moments and their gradients with respect to design variables can be readily obtained via polynomial chaos approach. However, the evaluation of the probabilities of the cost and constraint functions and their gradients, requires the integration over the range that corresponds to the failure region. Introducing a heaviside function in the integral that characterizes the probability of failure, the integration can be carried out over the fixed range of random variables. In order to alleviate the non-differentiable property of the heaviside function, a smooth approximation of the heaviside function is then utilized. Guidelines to assess the computational cost and solution accuracy of both intrusive and non-intrusive polynomial chaos approaches are presented. Numerical results for the shape optimization of a linear elastic structure demonstrate the effectivity of the approach. References [1] Eldred M. Design under uncertainty employing stochastic expansion methods. Interna- tional Journal for Uncertainty Quantification. 2011;1(2):119–146. [2] Maute K.,Weickum G., and Eldred M. A Reduced-Order Stochastic Finite Element Ap- proach for Design Optimization under Uncertainty. Structural Safety. 2009;31:450–459.

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Title: A Framework for the Characterization and Population Averaging of Full Mitral Valve Geometry

Author(s): Amir Khalighi, Andrew Drach, Chung-Hao Lee, Michael Sacks, *UT Austin*.

The Mitral Valve (MV) is the left atrioventricular valve preventing the backward flow of blood in the left atrium during ventricular systole. The MV complex is comprised of annulus, leaflets, chordae tendineae, and papillary muscles. The MV geometry has a significant impact on the valve competence and alterations in the geometry may lead to non-homeostatic conditions. The intra-individual variations and pathological alterations obscure the relation between the valve geometry and its physiological functionality. We present a novel methodology to analyze the entire MV geometry. We model leaflet geometry using a two-scale model which distinguishes dimensional variations (large-scale features) from the detailed shape variations (fine-scale features), and thus enables us to accurately characterize geometrical features of the leaflets and quantify them within an objective framework. The large-scale geometry was recovered using superquadrics surface fitting. For each valve, there are two surface meshes denoting the Atrial and Ventricular sides of the MV leaflets. The Levenberg–Marquardt non-linear programming algorithm was employed to determine the superquadratic fits. Next, we reconstruct features not captured by superquadratic model through Fourier reconstruction. A scalar field denoting the fine-scale features was defined based on the normal residual from the superquadrics surface. This field was then reconstructed by Conformal Fourier Transform method using Non-Uniform Fourier Transform (NUFFT) technique. Due to the irregular sampling of the input data, iterative NUFFT was used to prevent spectrum distortion. Through this geometry decomposition, we characterize the geometry of MV with a relatively small set of parameters. The proposed pipeline enables the reconstruction of leaflet geometry with an adjustable level of detail. Chordae tendineae structure is modeled by the medial axis representation with the skeleton reconstructed using NURBS and cross-sectional area variations assigned pointwise along the skeleton. The branched chordal structure is analyzed by the set of topological parameters. These parameters are different from the geometric parameters for the leaflet geometry due to the distinct morphological differences between two geometric structures. Chordal descriptors encode such geometric information as number and distribution of origins (chorda-papillary muscle attachment loci), density of branching points in chordal structure, and number and distribution of insertion points (chorda-leaflet attachment loci).The proposed framework is used to study dataset comprising of five ovine MV and develop a population-averaged geometric model of ovine MV. The averaged model is compared to the individual MV reconstructions and major modes of variation/similarity are discussed in detail.

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Title: Probabilistic Inference of Model Parameters and Missing High-Dimensional Data Based on Summary Statistics

Author(s): Mohammad Khalil, *Sandia Nat'l. Lab.*.

We present the results of an application of Maximum Entropy and Approximate Bayesian Computation methods to the probabilistic inference of model parameters in the absence of experimental data. The available published data are in the form of indirect summary statistics, being nominal values and error bars, of model parameters. This approach relies on generating data that is consistent with the given summary statistics. The methodology permits the forward propagation of parametric uncertainty through the computational model in a manner that is consistent with the published statistics. For the specific application to chemical modeling of hydrogen-air ignition, the previous algorithm consisting of a nested Markov Chain Monte Carlo procedure, with the outer chain exploring the missing data space and inner chain the unknown parameters, is computationally taxing given the high dimensionality of the missing data (in the order of 100s to 1000s). We propose an alternative approach consisting of importance sampling and Gauss–Hermite quadrature for parameter inference resulting in orders of magnitude speedup in data likelihood evaluation. Despite the strong nonlinearity in the model, the consistent data sets all result in nearly Gaussian conditional parameter probability density functions. Thus, the proposed technique based on importance sampling with a Gaussian proposal is adequate for parameter estimation in this investigation. A consensus joint posterior on the parameters is obtained by pooling the posterior parameter densities given each consistent data set.

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Title: The Signal-to-Noise Ratio Due to Biological Noise in Field-Effect Sensors Calculated Using the Stochastic Poisson Equation and Polynomial-Chaos Expansion

Author(s): Amirreza Khodadadian, *Vienna U. Tech.*; Clemens Heitzinger, *Arizona State U.; Vienna U. Tech.*.

Introduction. Nanowire field-effect bio- and gas sensors are an emerging sensor technology and, at the same time, an interesting model system for stochastic PDEs. We have introduced various PDE models to understand the functioning of these devices in the past. Here we include the randomness due to the biomolecules at the sensor surface and present a fast numerical approach. These results are useful to quantify noise and fluctuations in sensors and hence their detection limit. The model. The basic model equation here is the stochastic Poisson-Boltzmann equation. It describes the electrostatic interaction between the molecules at the sensor surface and the semiconducting transducer. The nonlinear Poisson-Boltzmann equation is more realistic, but the linearized equation is popular because of its simpler structure. The number of stochastic dimensions is large due to the large number of molecules. In previous works, we have calculated the orientation of the biomolecules from their electrostatic free energy. Their number at the surface is modeled as an association/dissociation process. The numerical approach. We use a polynomial-chaos expansion and basis adaptation. First, we determine the subdomain of the computational domain that is affected most by the random molecules. Then we project the potential on this subdomain onto the Gaussian chaos on the whole domain and construct the isometry for basis adaptation using the complete Gaussian component first and then with a Gram-Schmidt procedure. Finally, once the electrostatic potential is known, the concentrations of electrons and holes inside the transducer are calculated. Then the current through the sensor is calculated, which is the quantity of interest. The random movement of the molecules gives rise to noise in the transducer, which is quantified by the signal-to-noise ratio defined as the expected value of current over its standard deviation. In order to increase the signal-to-noise ratio, we numerically investigate the effects of doping concentration, oligomer length, surface charge, salt concentration, and the geometry of the transducer. Conclusions. We use polynomial chaos and basis adaptation in an efficient numerical algorithm for the calculation of noise and fluctuations in nanowire sensors. The basic model is the stochastic Poisson-Boltzmann equation: It relates the randomness of the molecules to the electrostatic potential, from which the quantity of interest, the current through the sensor, is calculated. The problem is computationally demanding due to the large number of stochastic dimensions.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Numerical Simulation of Some Coupled Processes of Mechanics of Porous Media

Author(s): Eduard Khramchenkov, Maxim Khramchenkov, *Kazan Federal U.*.

Mechanics of porous media is theoretical basis of such branches of science as rock mechanics, soil physics and so on. But at the same moment some complex processes in the geosystems lacks full theoretical description. The example of such processes is metamorphosis of rocks, catagenesi processes, and filtration process in swelling and unswelling soils, earth quakes and correspondent variations of stress-strain state. In such processes chemical transformation of solid and fluid components, heat release and absorption, phase transitions, rock destruction occurs. Extensive usage of computational resources in scope of traditional models of the mechanics of porous media cannot guarantee full correctness of obtained models and results. The process of rocks consolidation which happens due to filtration of underground fluids is described from the position of rock mechanics. As an additional impact, we consider the porous media consolidating under the weight of overlying rock with coupled complex geological processes, as a continuous porous medium of variable mass. The example of such processes is metamorphosis of rocks and correspondent variations of stress-strain state. In such processes chemical transformation of solid and fluid components, heat release and absorption, phase transitions, rock destruction occurs. In this work description of processes of mass exchange between fluid and poly-minerals material in porous media from various kinds of rocks (primarily sedimentary rocks) have been examined. It was shown that in some important cases there is a storage equation of non-linear diffusion equation type. In addition, process of filtration in un-swelling soils, swelling porous rocks and coupled process of consolidation and chemical interaction between fluid and particles material were considered. In the latter case equations of physical-chemical mechanics of conservation of mass for fluid and particles material were used. Finite difference method was used for discretization of the obtained system of equations. Regular cubic grid was constructed in the area of simulation. Linearization of non-linear coefficients was performed to obtain system of linear algebraic equations. Iterative calculations on each time step were conducted to obtain more stable solution. AMGCL computational library was used to perform fast computations on each time step. It is based on algebraic multigrid methods for preconditioning and provides effective realization of iteration solvers on the basis of OpenCL framework.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Subspace Methods for Multi-Physics Large-Scale Uncertainty Quantification

Author(s): Bassam Khuwaileh, Paul Turinsky, *North Carolina State U.*.

In conjunction with modern large scale nuclear reactor simulators, it is important to quantify the uncertainty in best estimate predictions. However, quantifying the uncertainty in multi-physics large scale applications often involves huge computational cost. Therefore, subspace based algorithms for large scale Uncertainty Quantification (UQ) problems have received considerable attention and have been explored as alternatives for reducing the computational burden associated with forward and adjoint UQ methods. Previous efforts explored the application of subspace methods to both linear and non-linear single–physics UQ problems, where the uncertainty is propagated linearly along the Degrees of Freedom (DoFs) with large uncertainty components. Moreover, Reduced Order Modeling (ROM) based goal-oriented surrogates have been used to replace the original models for non-linear uncertainty propagation using Monte Carlo sampling [1,2]. In this work, subspace based algorithms for linear and non-linear uncertainty propagation have been extended to large scale multi-physics applications. First, the previous algorithm for single-physics linear UQ was extended to multi-physics UQ problems. Results compare the performance of the proposed algorithm with that of the sandwich rule. Further, Monte Carlo forward UQ has beeb implemented and compared with a subspace based version of Monte Carlo based Uncertainty Quantification (MCUQ) proposed in this work. The proposed MCUQ approach depends on a biased Monte Carlo sampling approach which accelerates the convergence of the MCUQ algorithm. Finally, an efficient method for estimating the uncertainty contribution of each of the uncertainty sources has been implemented along with the MCUQ approach proposed here. All comparisons were performed for CASL VERA Progression Problem Number 2, which equates to a pressurized water reactor 2D fuel lattice. The TRITON analysis sequence (part of ORNL SCALE6.1 package) was used to simulate lattice behavior, including depletion effects. The uncertainty quantification was completed utilizing a new tool kit, the Reduced Order Modeling based Uncertainty/Sensitivity Estimation (ROMUSE), that is compatible with SCALE6.1. Our current work focus is on extending capabilities and applying to depletion problems with thermal-hydraulics feedback simulated using the CASL core simulator, VERA-CS. 1. Galbally, D., Fidkowski, K., Willcox, K., & Ghattas, O. (2010). Non■linear model reduction for uncertainty quantification in large■scale inverse problems. International journal for numerical methods in engineering, 81(12), 1581-1608. 2. Bang, Y. (2012). Hybrid Reduced Order Modeling Algorithms for Reactor Physics Calculations. PhD Dissertation, North Carolina State University.

13th U.S. National Congress on Computational Mechanics
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Title: A Natural Framework for Isogeometric Fluid-Structure-Interaction: Coupling BEM and Shell Models

Author(s): Josef Kiendl, Alessandro Reali, *U. Pavia*; Luca Heltai, Antonio DeSimone, *SISSA*.

We propose an FSI approach for the coupling of thin structures and viscous flow. Pursuing a “fully isogeometric” approach, both the structure and the fluid problem are completely described the CAD geometry, i.e., the NURBS surface model, which is made possible by using a shell formulation for the structure and a boundary integral representation for the fluid. We use a staggered approach solving the structural and the fluid problem separately. For structural analysis, we use a nonlinear isogeometric Kirchhoff-Love formulation, based on [1] and extended to the large strain regime. We derive the shell formulation consistently from the continuum model such that arbitrary 3D hyperelastic constitutive models can be employed [2]. The fluid is modeled by the 3D steady Stokes equation, which is solved by an isogeometric boundary element method. In particular, we use an isogeometric collocation boundary integral approach [3] that eliminates the singularities typically appearing in the boundary integrals. The advantage of the BEM approach is that volumetric meshing is avoided giving also the possibility to treat problems with an infinite computational domain. In the context of FSI, it additionally allows for a very natural coupling with the structure, where both fluid and structural model are discretized by the NURBS surface description of the design model. Several numerical tests demonstrate the efficiency and applicability of the proposed method. [1] J. Kiendl, K.-U. Bletzinger, J. Linhard, and R. Wüchner. Isogeometric shell analysis with Kirchhoff-Love elements. Computer Methods in Applied Mechanics and Engineering, 198 (2009) 3902–3914 [2] J. Kiendl, M.-C. Hsu, M. C. H. Wu, A. Reali. Isogeometric Kirchhoff-Love shell formulations for general hyperelastic materials. submitted (2015) [3] L. Heltai, M. Arroyo, A. DeSimone. Nonsingular isogeometric boundary element method for Stokes flows in 3D, Computer Methods in Applied Mechanics and Engineering 268 (2014) 514-539

13th U.S. National Congress on Computational Mechanics
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Title: Boundary Integral Formulation for Asymmetric Impinging Wall Jets with Arbitrary Nozzles

Author(s): Sung Sic Yoo, Do Wan Kim, *Inha U.*; Wing Kam Liu, *Northwestern U.*.

We present an efficient boundary integral formulation for solving two-dimensional impinging wall jets which has arbitrary nozzles. We assume that the jet emanating from an arbitrary nozzle impinges to a straight wall, and the flow is incompressible, irrotational, and inviscid. The point of this problem is to find the free boundary, the contacting surface between the flow and the surrounding air. The solution can be represented as the stream function and we can use a layer potential over the nozzle and free boundary. The free boundary is not known a priori and it is a part of the solution in this jet problem, which makes this problem highly nonlinear, and therefore hard to solve. For this reason, it is inevitable to devise an iterative algorithm. If a prescribed free boundary is given, then our formulation gives the direction toward the solution in a systematic way. We show the convergence of our method, provide examples for the reliability of numerical results, and finally illustrate the calculated solutions of the jets with arbitrary nozzles.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Effect of the Spatial Distribution of Voids on the Thermo-Mechanical Properties of Porous Media

Author(s): Sang-Yeop Chung, *Technische U. Berlin*; Ji-Su Kim, Tong-Seok Han, *Yonsei U.*.

The voids within the specimen strongly affect the physical properties of the material. The voids within a specimen have an important role in enhancing the thermal performance of the material, while the concrete strength decreases as the void ratio increases. Concrete is a heterogeneous material, and its material properties are affected by the spatial distribution of each constituent, e.g., cement and aggregate. In addition, concrete is a porous material and it contains numerous entrained voids inside a concrete specimen. The characteristics of concrete specimens can significantly differ due to the void clustering and anisotropic void distribution; therefore, a proper method for examining the spatial distribution of voids in concrete is necessary for better understanding of the material behavior. In this study, the effect of void clustering as well as anisotropic void distribution on the material properties of concrete, such as thermal conductivity and directional stiffness, are investigated. A set of virtual concrete specimens with different void clusters are generated. Then, the characteristics of the spatial distribution of voids in the specimens are investigated using probabilistic description methods, and the thermal and mechanical properties of the specimens are also examined using finite-element simulations. The simulation results demonstrate a relationship between the degree of void clustering and the thermo-mechanical properties of porous concrete specimen. The effect of anisotropic void distribution on the physical properties of porous media is also confirmed.

13th U.S. National Congress on Computational Mechanics
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Title: Environment Embedded Photoisomerization Model of Diarylethene

Author(s): Muyoung Kim, Jung-Hoon Yun, Maenghyo Cho, *Seoul Nat'l. U.*.

Among various photo responsive materials, diarylethene is regarded as most promising materials for its thermal stability, fatigue resistance, rapid and reversible change. Hence, diarylethene in crystalline phase has received great attention for its macroscopic deformation with light irradiation. Fundamental physics of the photo reactivity lies on the photoisomerization, which turns from open ring to closed ring isomer in UV light (cyclization) and turns back to open ring isomer when visible light is irradiated (cycloreversion).[1] Therefore, photoisomerization have been focused by many groups to examine molecular design for improving photochromic performance and identify isomerization mechanism to support experimental achievements. Nevertheless, less concern is shown on predicting quantitative isomerization progress under various light/thermal environments, which can bridge the gap between current academic use and industrial application. For this reason, we construct computational photoisomerization model which statistically estimates the photoisomerization as a population. The model is established by density matrix formalism with density functional theory calculation, and includes radiative physics by light and energy barrier crossing by thermal energy. Thus, the isomerization model provides time-evolutional population profile and its lagging under prescribed light/thermal condition. Based on the population data, we discuss fundamental physics of photo-switching and effect of environmental parameters on the isomerization. For applying the photochromic nature of target molecule, density functional theory calculation (geometry optimization, TDDFT, frequency calculation) derives energy path of population transition and photo-switching properties (energy level, electric transition dipole moment, vibrational frequency, and activation energy) that are substituted in the model. We verify the reliability of our model by comparison with transient absorption spectroscopy[2] using ultrafast pulse laser. To identify the laser irradiation condition, starting point of the population transition set to excited state of the initial isomer in the model. Time constant obtained from population profile is a key parameter for the comparison. It is expected that establishment of environment embedded model provides elementary information for multi-physics research, and help diarylethene be reached industrial application. [1] S. Kobatake, S. Takami, H. Muto, T. Ishikawa, and M. Irie, Nature , 446 (7137), 778-781 (2007). [2] Y. Ishibashi, T. Umesato, S. Kobatake, M. Irie, and H. Miyasaka, J Phys Chem, 116 (7), 4862-4869 (2012).

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Development of Deformable 3D Gap Element for Simulation of Asymmetric Thermal Behavior in Nuclear Fuel Rod

Author(s): Hyo chan Kim, Yong sik Yang, Dae ho Kim, Yang hyun Koo, *KAERI*.

A light water reactor (LWR) fuel rod consists of zirconium alloy cladding tube and uranium dioxide pellets with a slight gap between them. The tube is initially filled with helium gas, which fills the gap between the pellets and cladding tube. The accurate modeling of heat transfer across the gap between fuel pellets and the protective cladding is essential to understanding fuel performance, including cladding stress and behavior under irradiated conditions. To establish heat transfer model through gap in fuel performance code, gap conductance on the basis of the Ross and Stoute model was employed in the most of previous works. In that model, the gap conductance that determines temperature gradient within the gap is a function of gap thickness which is dependent on mechanical behavior. Recently, many researchers have been developing fuel performance codes based on finite element method (FE) to calculate temperature, stress and strain in 2D or 3D. The gap conductance model for FE can be challenging issue in terms of convergence and nonlinearity because the elements which are positioned in gap have different gap conductance and boundary conditions of gap vary at each iteration step. In this paper, the deformable 3D gap element has been proposed and implemented to simulate asymmetric thermo-mechanical fuel behavior. Thermo-mechanical 3D finite element module incorporating the gap element has been implemented using FORTRAN90. To evaluate the proposed 3D gap element, missing pellet surface (MPS) which results in asymmetric heat transfer in pellet and cladding was simulated. As a result, maximum temperature of pellet for MPS problem calculated with the specified 3D gap element is much higher than the temperature calculated with uniform gap conductance model that multidimensional fuel performance code employs. Higher temperature of pellet results in generation of large amount of fission gas release which increase rod internal pressure and high thermal strain of pellet that causes increase of cladding stress by pellet-cladding mechanical interaction (PCMI). The results demonstrate that 3D simulation is essential to evaluating temperature and stress of pellet and cladding for asymmetric geometry simulation. [1] MICHEL, B., SERCOMBE, J., NONON, C., FANDEUR, O., "Modeling of Pellet Cladding Interaction", Comprehensive Nuclear materials, Elsevier Ltd., Amsterdam (2012) 682-691. [2] HANSEN, G., A Jacobian-free Newton Krylov method for mortar-discretized thermo-mechanical contact problems, J. Computational Physics 230 (2011) 6546. [3] Steven Nesbit et al., Use of core analyses in assessments of fuel failure risk due to pellet-cladding interaction, ANFM 2009.

13th U.S. National Congress on Computational Mechanics
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Title: Multi-Scale Modeling of Heterogeneous Infrastructure Materials Subjected to Viscoelastic Deformation and Rate-Dependent Fracture

Author(s): Yong-Rak Kim, Taesun You, *U. Nebraska*; Jamilla Emi Sudo Teixeira, *U. Federal do Espírito Santo*; Flavio Souza, *Multimech R&D, Inc.*; David Allen, *Texas A&M Transport. Inst.*.

This study presents a multiscale computational model, along with its validation and calibration, to predict the damage-dependent behavior of multiphase infrastructure materials subjected to viscoelastic deformation and cracking. Two length scales (global and local) are two-way coupled in the model framework by linking a homogenized global scale to a heterogeneous local scale representative volume element (RVE). Based on the two-way coupled multiscaling and the use of the finite element technique incorporated with material viscoelasticity and cohesive zone fracture, the model approach can successfully account for the effect of geometric heterogeneity, material viscoelasticity, and damage accumulation due to cracks in the small scale RVE on the overall performance of larger scale mixtures or structures. Along with the brief theoretical model formulation, the multiscale model is validated and calibrated by comparing the model simulation results with experimental tests of three-point bending beam of particulate mixtures where material viscoelasticity, geometric heterogeneity, and rate-dependent cohesive zone fracture are involved. To further demonstrate the modeling features, the three-point bending beam is also subjected to cyclic loading to simulate fatigue damage. By altering the mixture's constituent properties, it shows that the two-way coupled multiscale model can properly capture material-specific and microstructure-dependent damage characteristics. The model presented in this paper is expected to drastically reduce time-consuming and expensive laboratory tests, which, when performed in the traditional manner, require many replicates and are limited to identify the cause of microstructural damage and failure of various heterogeneous solids including infrastructure materials.

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Title: Crack Propagation in Silicon Anode Used in Li-Ion Batteries Based on Li-Ion Concentration Profile of Two-Phase Lithiation

Author(s): Yong-Woo Kim, Tong-Seok Han, *Yonsei U.*.

Among the various types of anode materials, silicon elicits superior theoretical performance. However, the performance of silicon anodes decreases significantly after a few charge/discharge cycles. The cracks result in the silicon anode losing its electric connectivity. During the first charging cycle, crystalline silicon changes to amorphous silicon and crack propagation takes place because of changes in the volume of silicon. In this study, the crack propagation was investigated by employing a PPR potential-based cohesive model at all boundaries of continuum elements. The crack propagation in the silicon anode, which is a significant factor in relation to Li-ion battery capacity, was evaluated using the Li-ion concentration profile of two-phase lithiation and the cohesive zone model.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Multi-Scale Concurrent Material-Topology Optimization Using a Level-Set Method

Author(s): Peter Dunning, H. Alicia Kim, *U. Bath*.

Advances in additive manufacturing (AM) techniques are opening new possibilities for structural design. In particular AM removes most traditional manufacturing constraints allowing novel, more efficient designs to be explored. AM also has the potential to create structures at the micro-scale, allowing tailoring of material properties within a continuous structure. A multi-scale topology optimization method can take advantage of both of these strengths of AM. The idea is to formulate optimization at two scales: the macro-scale determines the overall topology of the structure and the micro-scale determines the material properties within the structure. We present a new framework for solving general multi-scale topology optimization problems. The aim is to fully exploit the potential of AM by allowing the micro-structure to vary within the macro-structure. Another key aspect of the method is that it can solve general problems and is not dependent on a particular problem definition. The first ingredient is to use homogenization to compute the effective material properties of the micro-structure. This forms a bridge between the scales, as the macro-scale material properties are dependent on the micro-scale design variables. The chain rule is used compute gradients of the macro-scale performance with respect to the micro-scale design variables. At this stage we could put all macro and micro design variables into a single problem and solve using a standard gradient-based optimizer. However, we want to allow the micro-structure to vary within the macro-structure, for example by defining a separate micro-structure for each element within the macro-structure domain. Also, single scale topology optimization problems usually have 1000’s of design variables. Therefore, the single problem solution approach to the multi-scale problem can become computationally prohibitive, especially for 3D problems. We propose an alternative solution strategy that naturally takes advantage of parallel computing by decomposing the problem. First, separate optimization problems are posed for the macro and each micro-structure. The key challenge is then to set appropriate constraint boundaries in the decomposed problems. This is overcome by introducing a constraint coordination method, which can be summarized as: 1) solve each problem with initial constraint boundaries, 2) perturb constraint boundaries and re-solve to estimate derivatives of the optimal objective value with respect to the constraint boundaries, 3) solve auxiliary optimization problems to obtain modified constraint boundaries, 4) check for convergence, otherwise return to step (1). The proposed strategy is used with a level-set topology optimization method to solve various multi-scale structural problems.

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Title: Temporal and Spatial Multi-Scale Simulation of Nanoindentation Using Hyper-QC

Author(s): Woo Kyun Kim, *U. Cincinnati*; Ellad Tadmor, *U. Minnesota*.

Over the past decades atomistic simulations such as molecular dynamics (MD) have made significant contributions to modeling materials by providing direct access to atomic-scale mechanisms which cannot be observed experimentally. Furthermore, atomistic simulations have been indispensable in developing predictive models for material properties and responses based on the fundamental understanding of atomic-level processes. However, even with the aid of high-performance computing available today, the length and time scales of systems that can be modeled by atomistic simulations are by several orders of magnitude different from those of macroscopic systems of technological interest. Recently, Kim and Tadmor with their coworkers have developed a novel multiscale method, called hyper-QC, which can extend both length and time scales simultaneously [1]. Hyper-QC combines quasicontinuum (QC), a spatial multiscale method, and hyperdynamics, an accelerated MD scheme, on a single platform. In this talk, the hyper-QC simulation results of nanoindentation of a thin nickel film will be presented. Nanoindentation is the small-length scale counterpart to the conventional indentation test on macroscopic length scales used to measure hardness. Although the plastic deformation observed in macroscopic indentation tests is well-understood, the deformation mechanisms in nanoindentation tests are an ongoing area of research. Nanoindentation has been widely investigated using fully-atomistic schemes such as MD. However, due to the short time scale problem, most MD simulations are performed at indentation rates that are many orders of magnitude faster than those used in actual experiments. Hyper-QC enables the simulation at the indentation rates up to three orders of magnitude lower than that of the conventional MD scheme. Moreover, a novel bias potential for hyperdynamics using the slip mechanism of fcc crystals that is computationally less expensive than the originally proposed bias potential using the eigenvalue/eigenvector of the Hessian will be introduced. [1] Kim, W. K.; Luskin, M.; Perez, D.; Voter, A. F.; Tadmor, E. B.: Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. J. Mech. Phys. Solids 2014, 63, 94-112.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Smoothed Finite Elements of Polyhedral Shape

Author(s): Hobeom Kim, Chan Lee, Seyoung Im, *KAIST*.

In this study, three-dimensional polyhedral elements based on smoothed finite elements method (S-FEM) are studied. The S-FEM by means of the gradient smoothing improves the accuracy, the efficiency and the convergency of solutions. Furthermore, it makes it possible to obtain a quality solution despite severe mesh distortion. S-FEM is categorized into cell-based smoothed FEM (CS-FEM), node-based smoothed FEM (NS-FEM), and edge-based smoothed FEM (ES-FEM) depending on how to construct smoothing domain. Unlike the conventional FEM, S-FEM is capable of accommodating polyhedral elements naturally due to the gradient smoothing technique. The performance of CS-FEM, NS-FEM and ES-FEM using polyhedral elements is compared with one another. Especially for the case of hexahedral elements, the performance of each methods is compared with the conventional FEM. Numerical examples show the ES-FEM leads to efficient and accurate solutions for various linear elasticity problems and NS-FEM has superior volumetric-locking property for nearly incompressible materials. As reported previously, the present formulation yields polyhedral finite elements that are not sensitive to element distortion, and the stiffness formation is more efficient and straightforward.

13th U.S. National Congress on Computational Mechanics
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Title: Energy-Conserving Variable-Node Interface Elements for Interaction Analysis

Author(s): Jungdo Kim, Seyoung Im, *KAIST*; K. C. Park, *U. Colorado-Boulder*.

A new algorithm is proposed to achieve the energy conservation of discrete systems with non-matching interfaces. In a variable-node construction of nonmatching interfaces, additional interface degrees of freedom often need to be created, which means that each time additional interface nodes are added, the system becomes essentially a different discrete system. This is because, even though the resulting discrete system may vary from time to time, its continuum counterpart should remain the same throughout the analysis. The present paper presents an energy conserving strategy when the system nodes vary for each of the partitions. This has been realized by requiring that both the kinetic and strain energy of the new system at the start of the next step should be the same as the final condition of the preceding discrete system. The present energy-conserving strategy is demonstrated via several examples including linear dynamic and FSI problems using smoothed finite element method, which provides a convenient framework for transforming nonmatching meshes into matching mesh by introducing variable-node elements.

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Title: Crystal Plasticity Analysis of HCP Polycrystals

Author(s): Ji Hoon Kim, *Pusan Nat'l. U.*; Joo-Hee Kang, Chang Dong Yim, Chang-Seok Oh, *KIMS*; Myoung-Gyu Lee, *Korea U.*.

Crystal plasticity finite element method is a useful tool for studying the behavior of polycrystals. Metals having HCP structure exhibit unique deformation behavior caused by the activation of multiple slip systems and twinning systems. Therefore, it is usually difficult to determine the constitutive relationships corresponding to the slip or twinning systems. In this work, in order to obtain the constitutive relationships of HCP polycrystals, the deformation of the oligo-crystals of the magnesium alloy AZ31B was analyzed experimentally and numerically. The tensile specimen of the oligo-crystal was prepared from the AZ31B ingot. The initial grain orientation map of the whole specimen was obtained by merging orientation maps taken by the orientation imaging microscope (OIM). Then, the tensile loading was applied to the specimen while the strain distribution was captured using the digital image correlation method. The finite element model of the oligo-crystal specimen was generated using the grain orientation information, and the deformation of the specimen under tensile loading was calculated and compared with experiments for obtaining the constitutive relationships at the crystal level.

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Title: Grain-Size Dependent Young's Modulus and Poisson's Ratio of Bulk Nanocrystalline Materials

Author(s): Tae-Yeon Kim, *Khalifa U. Sci.*; John Dolbow, *Duke U.*; Eliot Fried, *Okinawa Inst. Sci. & Tech.*.

We present a numerical study of the elastic properties of bulk nanocrystalline materials based on a continuum model introduced by Fried and Gurtin [1]. For nanoscale polycrystalline elasticity, the model gives rise to a balance equation that is fourth-order in the displacement field and that captures length-scale effects and accounts for interactions across grain boundaries via interface and junction conditions. To explore the properties and utility of the model, we developed a relatively inexpensive, non-conforming fi nite-element method based on C0-continuous basis functions (Kim et al. [2]). We introduce the variational form of the method that weakly enforces continuity of derivatives of the displacement fi eld across interelement boundaries and achieves stabilization via Nitsche's method. Based on the method, numerical studies are performed for a polycrystal subject to an uniaxial deformation. The distribution of the effective stress shows that the model captures high strain gradients in the vicinity of the grain boundaries and triple junctions. We examine the influence of the grain-size and the gradient length scale ■ which represents the length-scale effect at nanoscale. The effective Young's modulus decreases and the effective Poisson's ratio increases with increasing ■ and decreasing grain-size. This is because the length-scale effects and interactions across grain boundaries become significant with increasing ■ and decreasing grain-size. Numerical results are compared with experimental results for nanocrystalline copper. The model predicts a lower Young's modulus for nanocrystalline copper than for conventional coarsely-grained polycrystalline copper. The result shows about a 5% reduction of the effective elastic modulus for nanocrystalline copper and it compares favorably with experimental results. References [1] E. Fried and M.E. Gurtin, Gradient nanoscale polycrystalline elasticity: intergrain interactions and triple-junction conditions, Journal of the Mechanics and Physics of Solids, 57 (2009), 1749-1779. [2] T.-Y. Kim, J.E. Dolbow, and E. Fried, Numerical study of the grain-size dependent Young's modulus and Poisson's ratio of bulk nanocrystalline materials, International Journal of Solids and Structures, 49 (2012), 3942-3952.

13th U.S. National Congress on Computational Mechanics
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Title: Structural Origins of the Non-Linear Mechanical Response of Fibrin Networks Under Compression

Author(s): Oleg Kim, Mark Alber, *U. Notre Dame*; Rustem Litvinov, John Weisel, *U. Pennsylvania* .

Fibrin is a protein polymer that forms a three-dimensional viscoelastic scaffold of physiological blood clots as well as life threatening pathological thrombi. Despite the fact that compressive deformation of clots and thrombi is inherent to a number of (patho)physiological conditions, structural and mechanical changes of fibrin networks and their origins are largely unknown. The aim of this talk is to describe recently established correlations between structural changes and mechanical responses of fibrin networks exposed to compressive forces. Namely, our rheological measurements revealed nonlinear changes in network viscoelastic properties under compression. Using confocal microscopy, these non-linear mechanical properties were shown to originate from structural rearrangements of the entire fibrin network, as well as alterations of individual fibers including fiber buckling, bending and reorientation. We have quantified structures of the fibrin networks and their rheological properties and demonstrated that the softening of the network occurred as a result of buckling and bending of individual fibers upon compression [1]. The network hardening strongly correlated with an increase in the number of intersecting fibers resulting from densification of the compressed network. Our results suggest a complex interplay of entropic and enthalpic contributions accompanying structural and mechanical changes in fibrin networks under compressive loads. These findings provide first direct evidence of the structural origins of fibrin clot mechanical response to compressive. We are currently developing and calibrating multi-scale computational model to study clot deformations in response to variety of different types of loads. Predictive simulations can lead to alteration of fibrin properties which may potentially provide means for development of design principles for enhanced biomaterials and intervention into thrombosis. 1. Oleg V. Kim, Rustem I. Litvinov, John W. Weisel and Mark S. Alber [2014], Structural basis for the nonlinear mechanics of fibrin networks under compression, Biomaterials 35, 6739-6749.

13th U.S. National Congress on Computational Mechanics
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Title: Turbulent Bubbly Flow Under Breaking Water Waves

Author(s): James T Kirby, Morteza Derakhti, *U. Delaware*.

Wave breaking is a highly dissipative process, representing an important source of turbulence in the ocean surface layer. Air is entrained and rapidly evolves into a distribution of bubble sizes which interact with fluid turbulence and organized motions. This interaction, especially during active breaking, enhances liquid velocity fluctuations, reduces the energy in large scale motions, increases the energy of small scale motions, enhances dissipation, and may alter wave-induced vortex structures. We describe recent efforts to examine bubble-mediated dissipation rates and transport processes in breaking events in a range of water depths, from intermediate/deep water breaking triggered by high local wave steepness, to depth-limited breaking in the shallow water surfzone. We use a 3D Navier-Stokes solver with VOF interface tracking, incorporating bubble populations using a continuum Eulerian-Eulerian formulation for a poly-disperse bubble phases. Turbulence is simulated using a LES approach with Germano/Lilly dynamic Smagorinsky subgrid formulation. SGS bubble-induced turbulence is modeled using a well known formulation of Sato and Sekoguchi. We examine non-stationary turbulence structure, momentum exchange between dispersed bubbles and liquid phase, bubble effects on the mean and turbulent field, shear- and bubble-induced dissipation, bubble void fraction distribution and integral properties of the bubble plume both in spilling and plunging breakers. We study the process both during active breaking which turbulence is generated, bubbles are entrained and there is a strong interaction between fluid and dispersed bubble phase as well as post breaking field up to 22 wave periods after breaking. Comparison of mean and turbulent velocities, void fraction distributions and integral properties of the bubble plume with experimental data show that the model is capable of capturing the large scale of turbulence and bubble plume kinematics and dynamics fairly well, and the inclusion of bubbles gives better results in terms of total dissipation and turbulent velocities. In addition, the relative importance of preferential accumulation of dispersed bubbles in coherent vortex cores is investigated. We investigate the formation and evolution of breaking-induced turbulent coherent structures (BTCS) under both plunging and spilling waves as well as BTCS's role on intermittent 3D distributions of bubble void fraction. The vertical transport of dispersed bubbles by downburst type coherent structures in the transition region is compared to that by obliquely descending eddies.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A New Approach for Stress-Based Topology Optimization Problems for Multi-Layer Composite Shell Structures

Author(s): Cesar Kiyono, Emílio Silva, *U. São Paulo*; Junuthula Reddy, *Texas A&M U.*.

This work presents a new approach for handling stress-based topology optimization problems applied to multi-layer composite shell structures made of isotropic and orthotropic materials. Material distribution is optimized in order to minimize the maximum stress value at the entire structure. Specific failure criteria are evaluated for different materials and the safety factor is calculated to normalize the failure criteria values. This safety factor is the maximum coefficient that can be multiplied to the actual loads while the failure criteria are still satisfied [1]. Thus, the main objective of this work it to maximize the minimum safety factor value, and consequently, the maximum stress value is minimized, subjected to a volume constraint to prevent fully-covered domains. To find the minimum safety factor value, the p-norm formulation is used. However, when using a small value of the p-norm penalization coefficient (4 or 6), the p-norm function does not estimate well the minimum safety factor value, and thus, stress concentration can occur [2]. On the other hand, if the p-norm penalization coefficient is large (12 or larger), the minimum safety factor value is well estimate by the p-norm function, however, it can generate a discontinuity between iterations because of the local nature of the stress. Thus, we propose the multi-p-norm objective function to prevent both problems, which is the product of p-norm functions using different penalization coefficients. Furthermore, SIMP and qp-relaxation approach [3] are used in the formulation as the material model, and the GCMMA algorithm as the optimization solver. We also propose use the continuation method to both p and q coefficients to improve the convergence of solutions. To illustrate the proposed approach, examples of multi-layer shell structures with isotropic and orthotropic materials subjected to in-plane and out-of-plane loads are considered.
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13th U.S. National Congress on Computational Mechanics
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Title: A Multi-Tiered Approach to UQ in High-Dimensional Uncertainty Spaces

Author(s): Richard Klein, Don Lucas, Vera Bulaevskaya, Gardar Johannesson, Peer-Timo Bremer, David Domyancic, Scott Brandon, *LLNL*.

I will describe research in four areas that when taken together hold the promise of providing a robust attack on the curse of dimensionality of the high dimensional uncertainty spaces common in highly coupled, non-linear, and multi-scale physics applications. These areas are: (i) enhancements to approaches to adaptive sampling by aggregation. Given the complexity of a physical system it is not known in advance which of many choices for adaptive sampling are optimal for problems of high dimensional uncertainty. Aggregation provides a path toward adaptive sampling optimization; (ii) Topological characterization of high dimensional spaces and extraction of lower dimensional manifolds to aid in adaptive sampling; (iii) Regularized regression for dimensional reduction of high dimensional spaces and (iv) advances in our UQ Pipeline to accommodate extreme size ensembles on current and emerging computational architectures. We have developed robust adaptive sampling approaches by aggregating and combining the feedback from multiple strategies that obviate the need to know in advance which particular methodology is best for a given response. We extend this methodology through multi-variate sampling with Learning-based Expected Improvement. We have developed topological UQ techniques that yield insights into the structure of high dimensional functions through topological analysis and visualization. The approaches are based on Morse-Smale decomposition and allow us to embed topological structures into lower dimensional manifolds while providing feedback to adaptive samplers. Statistical methods from the fields of sparse signal recovery and network graph theory are being used to determine the relevant features, dimensions, and connections in extreme-scale UQ datasets. L1-penalized regression is used to ■t high-order/high-dimensional models of ensemble variance for highly under-determined systems, and the models are then represented as network graphs. Important cliques and connections in the graphs are measured and used to guide subsequent sampling and analysis. These approaches have been applied to systems containing as many as O(100) parameter dimensions. The LLNL UQ Pipeline has been successfully used to generate tens of thousands of ensemble simulations on Petascale platforms. However, the current hardware and operating system limitations are a hindrance to performing larger ensemble studies needed for very high dimensional UQ studies. A new tool developed at LLNL has the ability to run 1.5 million simultaneous jobs –one per core – on Sequoia. Implementing this tool within the UQ Pipeline will allow us to conduct UQ studies at much larger scales on current and upcoming multi-petaflop platforms.

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Title: An Improved Enriched Finite Element Method for Hydraulic Fracturing Propagation

Author(s): Denis Klimenko, Arash Dahi Taleghani, *Louisiana State U.*.

A novel enrichment formulation is presented for modeling coupled fluid-driven fracture propagation. The proposed method is based on the extended finite element method with modifications to incorporate variable stress singularity at the crack tips to account for the transition between toughness-dominated and viscous-dominated regimes. These enrichment functions are inspired by the asymptotic analytical solutions. Additionally, a consistent enrichment function is introduced for fluid pressure close to the fracture tip. To validate the proposed method, the numerical results are compared with the analytical solutions for two extreme propagation regimes. A superconvergent method is also proposed to calculate the energy release rate at the fracture tips for the general variable singularity. Mesh independency of the proposed method is verified and the convergence with the rate of 0.58 has been achieved for the couple model using this method. The shear lag approximation is utilized to incorporate the height effect into the proposed method to describe the evolution of the fracture geometry more realistically. The proposed method does not require high mesh concentration at the tip regions to achieve high numerical accuracy and is fully parallelized to expedite computation. High numerical accuracy with short execution time is crucial for simulating complicated geometries such as interacting hydraulic fractures or interaction a hydraulic fracture with pre-existing natural fractures. Hence, an example of fracture propagation in presence of multiple pre-existing fractures is presented to show a successful application of the model for predicting fracturing performance in Barnett Shale.

13th U.S. National Congress on Computational Mechanics
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Title: Morphological Transitions of Macromolecular Aggregates

Author(s): Luigi Perotti, Sanjay Dharmavaram, Joe Rudnick, Robijn Bruinsma, William Klug, *UCLA*.

Biological macromolecules (e.g., lipids and proteins), can self-assemble to form super-structures, or aggregates, which are often highly symmetric. These structures also commonly exhibit functional changes in morphology, which can be driven by local conformational changes of the assembly units, or microstructural rearrangements. We will present theory and simulations that model these transitions using the framework of differential growth, large deformation elastoplasticity, and the Landau theory of structural phase transitions in solids. Applying the models to viruses that infect bacteria and extremophile archaeal cells, we will show how structural mechanics and the kinetics of crystalline defects can control the morphological changes (stretching, bending) of macromolecular shells.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Computational Framework for Scale-Bridging in Multi-Scale Simulations

Author(s): Jaroslaw Knap, *Army Rsch. Lab.*.

Over the last few decades, multi-scale modeling (MSM) has become a dominant paradigm in materials modeling. The practical impact of MSM depends, to a great extent, on its ability to utilize modern computing platforms. However, since there are no general computational frameworks for MSM, the vast majority of multi-scale material models or simulations are developed on a case-by-case basis. We seek to formulate an adaptive computational framework for scale-bridging in MSM. We do not plan to develop a specific method for MSM simulations, but instead, aim to develop a broad and flexible numerical framework for designing and developing such simulations. Our focus is primarily on new scalable numerical algorithms applicable to a wide range of MSM applications. These algorithms fall into one of the three areas: i) scalable data transfer between parallel applications, ii) adaptive strategies for MSM, and iii) data analytics for MSM. We present a formulation of our computational scale-bridging MSM framework. Subsequently, we describe development of a two-scale multi-scale model of composite materials, as well as, evaluate its performance for a complex, real-life application.

13th U.S. National Congress on Computational Mechanics
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Title: Computation of Free Surface Flow with Transversely Oscillating Cylinder

Author(s): Serpil Kocabiyik, Oleg Gubanov, *Memorial U. Newfoundland*.

The major technical issue encountered in the solution of free surface problems is the appearance of numerical instabilities that arise due to the description of the mesh movement to track the moving boundaries, non-linearity of the governing equations and boundary conditions implementation at the free surface and rigid body surface. In the present computational model, a fluid flow governed by the full Navier-Stokes equations is only modeled within a two-dimensional computational domain. The motion of the air is neglected and the effect of the ambient pressure exerted on the fluid by the air is taken into consideration. The method of solution is based on a finite volume discretization of the unsteady Navier-Stokes equations in their pressure-velocity formulation on a fixed Cartesian grid. A special integral form of the governing equations is derived by extending the Reynolds transport theorem and then applying it to control volumes containing a fluid interface. The combined volume of fluid and fractional area/volume obstacle representation method, and the cut cell method are employed to track the fluid-air and fluid-body interfaces. A sparse linear system in pressure and velocity components is solved by using the generalized minimal residual method with ILUT preconditioner to advance the simulation of unsteady flow in time. Creative use of object oriented programming, data abstraction and template metaprogramming paradigms enables us to implement principle computational fluid dynamics concepts, directly, into the computer code developed in this study. The numerical simulation tool is applied to the problem of unsteady, laminar, two-dimensional flow of a viscous incompressible fluid past a transversely oscillating circular cylinder in the presence of a free surface. The code validations are presented in special cases and good comparisons with previous experimental and numerical results are obtained. References: [1] E. Aulisa and S. Manservisi and R. Scardovelli and S. Zaleski (2003) ``A geometrical area-preserving volume-of-fluid advection method'', J. Comp. Physics, Vol. 192, pp. 355-364. [2] M. Brons, M. C. Thompson, T. Leweke and K. Hourigan (2014) ``Vorticity generation and conservation for two-dimensional interfaces and boundaries'', J. Fluid Mech., Vol.758, pp. 63-93. [3] P. Reichl, K. Hourigan and M. C. Thompson (2005) ``Flow past a cylinder close to a free surface'', J. Fluid Mech., Vol. 533, pp. 269-296.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Fully Non-Local QC Investigation of Microstructural Defects and Interfaces

Author(s): Dennis Kochmann, Jeffrey Amelang, Ishan Tembhekar, Gabriela Venturini, *Caltech*.

We present results obtained from a fully non-local formulation of the Quasicontinuum (QC) method which is based on a new set of summation rules that minimize energy approximation errors and spurious force artifacts. To this end, the new, optimal summation rules require a set of sampling atoms (different from the representative atoms) to approximate the total Hamiltonian. This formulation, similar in spirit to quadrature rules, allows for automatic model adaption and provides high levels of efficiency in three-dimensional QC simulations. In addition, we use a new adaptation scheme which locally re-maps atomic neighborhoods so that the QC model can accurately represent large atomic motion, e.g. during plastic events and microstructure formation. The fully-nonlocal QC scheme is applied to three-dimensional examples of nanoscale plasticity, which emerge from interfaces, boundaries and defects in crystalline systems.

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Title: WebCL-Based Online Skin Lesion Border Detection for Dermoscopy

Author(s): James Lemon, Tansel Halic, *UCA*; Sinan Kockara, .

Dermoscopy is a highly effective and noninvasive imaging technique used in diagnosis of melanoma and other pigmented skin lesions. Many aspects of the skin lesion under consideration are defined in relation to the lesion border. This makes border detection one of the most important steps in dermoscopy image analysis. In current practice, dermatologists often delineate borders through a hand drawn representation based upon visual inspection. Due to the subjective nature of this technique, intra- and inter-observer variations are common. Because of this, the automated assessment of lesion borders in dermoscopy images has become an important area of study. Previous research indicates that one of the highest accuracy rates can be achieved using density based clustering techniques for skin lesion border detection. While these algorithms do have unfavorable computation time, we found this effect could be mitigated when implemented in parallel. This study presents a parallel implementation of a prominent density based skin lesion border detection (DBSLBD) algorithm for heterogeneous computing platforms. Heterogeneous computing refers to parallel programming for various device architectures such as multi-core CPUs, GPUs, and fully-integrated Accelerated Processing Units (APUs) etc. In this study, DBSLBD's computation steps have been carefully redesigned to run very efficiently on the heterogeneous platforms by transforming DBSLBD into a series of highly regular and independent concurrent operations. For this, we used WebCL, an emerging technology that enables a HTML5 Web browser to execute code in parallel on a variety of devices. All data structures are created to efficiently benefit from available memory hierarchies. How these structures reformed and represented in various memory hierarchies is illustrated.

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Title: Microstructure and Shape Optimization of Porous Biomedical Co-Cr-Mo Alloy Fabricated by Electron Beam Melting

Author(s): Yuichiro Koizumi, Arata Okazaki, Akihiko Chiba, *Tohoku U.*.

Electron beam melting (EBM) is an additive manufacturing (AM) method which has been applied to bio-medical implants. In addition to the manufacturing of customized implants, fabricating porous structure is attracting attention. Porous metals have low Young's modulus close to that of living bone are expected to avoid the stress-shielding which may decrease the density of bone surrounding the implants. The aim of this study is to develop porous biomedical titanium and Co-Cr-Mo (CCM) alloy with high strength and low Young's modulus taking advantage of the free form fabrication ability of AM technology combined with the shape optimization designing technology. Moreover, the influences of microstructures on mechanical properties and the formation mechanism of microstructure in porous structure fabricated by EBM were examined. Contrary to the previously reported microstructures of bulk CCM alloys fabricated by AM, which composed of columnar grain with strong <100> texture, unique microstructures with characteristic morphology was observed in EBM-built porous structures similarly to that observed on the surface of bulky EBM build parts. This was attributed to the difference in the crystal growth due to the fact that the inner region and the outer region of each 2D layer were melted by electron beam scanned with two different conditions called "hatch" and "contour", respectively. The unique microstructures in porous structure were regarded as the result of the process in which almost entire areas were melted by electron beam scanned with the contouring condition. Porous Co-Cr-Mo alloy with inverse body centered cubic (IBCC) structures were fabricated by EBM. These yield strength tend to increase with increasing Young's modulus. The porous structures was re-designed by structural optimization, targeting the increase in yield strength and the decrease in low Young's modulus simultaneously. Shape optimization based on traction method was carried out under the condition of minimizing maximum von Mises stress, controlling Young's modulus while maintaining constant volume fraction. Changes in Young's modulus of porous structure are relatively in good agreement with those expected, but the strengths were lower than expected. The effect of heat treatment was tested using the IBCC porous structure. After the heat treatment, strength was improved. However, Young's modulus increased significantly at the same time, probably because the columnar grain with <100> texture with lower Young's modulus changed to random oriented grains. This strongly suggests that the shape optimization taking the crystal orientation into account is important to control the mechanical properties of EBM built parts.

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Title: Scalable High-Order ALE Simulations

Author(s): Robert Anderson, Thomas Brunner, Veselin Dobrev, Ian Karlin, Tzanio Kolev, Robert Rieben, Vladimir Tomov, *LLNL*.

The Arbitrary Lagrangian-Eulerian (ALE) framework forms the basis of many large-scale multi-physics codes, and in particular those centered around radiation diffusion and shock hydrodynamics. Current ALE discretization approaches consist of a Lagrange phase, where the hydrodynamics equations are solved on a moving mesh, followed by a three-part ``advection phase'' involving mesh optimization, field remap and multi-material zone treatment. While traditional low-order ALE methods have been successful at extending the capability of pure Lagrangian methods, they also introduce numerical problems of their own including breaking of symmetry, and lack of energy conservation. In this talk, we present a general high-order finite element discretization framework that aims to improve the quality of current ALE simulations of radiation-hydrodynamics, while also improving their performance on modern data-centric computing architectures. We use the de Rham complex to guide the discretization of different physics components. In particular, kinematic quantities (e.g. velocity, position) are discretized with continuous (H1) finite elements, thermodynamic quantities (e.g. internal energy) use continuous (L2) elements, while H(div)-conforming finite elements are used for the fluxes in radiation diffusion. Our Lagrangian hydrodynamics algorithm is based on Galerkin variational formulation of momentum and energy conservation using the high-order de Rham finite elements. The use of high-order position description enables curvilinear zone geometries allowing for better approximation of the mesh curvature, which develops naturally with the flow. The remap phase of ALE is posed as an advection problem in artificial pseudo-time, describing the evolution of the post-Lagrangian mesh into the improved new mesh. This is discretized using a finite element Discontinuous Galerkin (DG) approach on high-order curvilinear meshes. The semi-discrete DG method results in high-order accuracy for sufficiently smooth fields, but can produce non-monotonic results for discontinuous fields. We consider several non-linear approaches to enforce monotonicity, including high-order algebraic Locally Scaled Diffusion (LSD), Flux Corrected Transport (FCT) and Optimization Based Remap (OBR). The ALE evolution of different materials in our framework uses high-order "material indicator" functions, and we have developed high-order closure models to model the sub-zonal material behavior during the Lagrangian phase. We have started exploring approaches for discretizing high-order multi-group radiation diffusion on general curvilinear grids and will report some initial results on the coupling with the high-order hydrodynamics. We will also present numerical tests illustrating the robustness and scalability of our discretization algorithms and discuss recent work to further improving their performance on modern architectures. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, LLNL-ABS-667265.

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Title: Adaptation Strategies for Discontinous Galerkin by Means of Tau-Estimation

Author(s): Moritz Kompenhans, Gonzalo Rubio, Esteban Ferrer, Eusebio Valero, *U. Politécnica de Madrid*.

The Euler and Navier Stokes equations have been discretized using a Discontinuous Galerkin Spectral Element Method (DGSEM). A low storage Runge-Kutta time integration scheme of order three was implemented and the mortar element method was applied to couple the element faces when hanging nodes or elements with varying polynomial orders are used in the computational mesh [1]. The advantage of the proposed method is the possibility to perform automatic local adaptation (using p refinement) based on tau-estimation. A mesh adaptation algorithm, based on the truncation error estimation by means of tau-estimation, was developed by Fraysse et al. for Finite Volumes, resulting in a very efficient and cheap adaptation sensor [3]. The tau-estimation method was successfully extended from low to high order methods by Rubio et al. [2] and finally a complete adaptation strategy is presented here. The adaptation scheme determines the polynomial order in each element based on the value and the rate of convergence of the truncation error. Furthermore the truncation error estimation permits the decoupling of the polynomial order in each spacial dimension which optimizes the computational cost. The adaptation algorithm developed is compared to other adaptation algorithms found in the literature. The adaptation techniques were tested and validated with different test cases. A full analysis of scaling regarding computational cost and required resources was performed. [1] D. A. Kopriva. Implementing Spectral Methods for Partial Differential Equations: Algorithms for Scientists and Engineers. Springer Publishing Company, 1st edition, 2009. [2] G. Rubio, F. Fraysse, D. A. Kopriva, and E. Valero. Quasi-a priori trun- cation error estimation in the DGSEM. Journal of Scientific Computing, pages 1–31, 2014. [3] F. Fraysse, J. de Vicente, and E. Valero. 2012. The estimation of truncation error by tau-estimation revisited. J. Comput. Phys. 231, 9 (May 2012), 3457-3482.

13th U.S. National Congress on Computational Mechanics
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Title: Robustness of Nodal Discontinuous Galerkin Spectral Element Methods for Conservation Laws

Author(s): David Kopriva, *Florida State U.*.

To get accurate solutions to fluid flow problems one can use high order approximations (e.g. 4 to 20). High order methods have great promise, especially their potential for greatly improved computational efficiency when compared to low order methods. Unfortunately, positive features of high order discretizations, especially low dissipation, mean high order methods often lack the robustness needed for industrial level computations. In this talk, I discuss how to devise provably stable high order methods. In particular, I present a skew-symmetric nodal DG spectral element method that is conservative, free-stream preserving and provably stable for curved elements and investigate effects of the variable geometric terms that arise when approximating conservation laws on curved elements.

13th U.S. National Congress on Computational Mechanics
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Title: Dynamically Coupled Fluid-Structure Interaction and Damage Model for Fatigue Prediction in Composite Structures

Author(s): Artem Korobenko, Xiaowei Deng, Jinhui Yan, Yuri Bazilevs, *UC San Diego*.

A large-deformation, isogeometric rotation-free Kirchhoff–Love shell formulation is equipped with a fatigue model for fully reversed cyclic loading to efficiently and accurately simulate fatigue failure in composite structures. The fatigue model developed in [1] is based on coupled approach of residual stiffness and strength. Stiffness degradation is represented as change of damage variable per loading cycle where the damage growth law is established in a form of damage initiation and damage propagation functions. To integrate equations for damage growth, the cycle jump technique is applied. The computations are done for a certain set of fatigue loading cycles at appropriately chosen intervals and the effect of stiffness degradation is extrapolated over corresponding intervals in an accurate manner. The model has been applied to simulate a fatigue failure of the CX-100 wind turbine blade that was fatigue loaded until failure using a hydraulic displacement excitation technique in National Renewable Energy Laboratory (NREL). The model is updated in a dynamic manner at several points during fatigue loading using sensor data. The final failure as well as stress redistribution due to stiffness degradation in damaged zones is captured in the experimentally-predicted number of loading cycles. Additionally the fatigue damage model is incorporated in full-scale FSI simulations of wind turbine blades in real operating conditions. [1]. W. Van Paepegem and J. Degrieck (2002). "A New Coupled Approach of Residual Stiffness and Strength for Fatigue of Fibre-reinforced Composites", International Journal of Fatigue, 24(7), 747-762

13th U.S. National Congress on Computational Mechanics
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Title: Theory and Algorithms for PDE-Constrained Optimization Under Uncertainty

Author(s): Drew Kouri, *Sandia Nat'l. Lab.*.

Many engineering and scientific application problems require the control or design of physical systems governed by partial differential equations (PDEs). These control and design problems are often formulated as large-scale PDE-constrained optimization problems. Moreover, the inputs to the PDE (for example, coefficients, boundary conditions, or initial conditions) are unknown and estimated from experimental data. For high-consequence applications, solutions to the original optimization problem must be 'resilient' to this input uncertainty. In addition, the numerical solution of such problems often requires an enormous number of samples of the input uncertainties to accurately characterize their effects. This results in an enormous number of forward simulations of a (computationally expensive) deterministic PDE at every optimization iteration. In this talk, I will discuss the mathematical theory for the solution of risk-averse PDE-constrained optimization problems. I will discuss the notion of risk measures and the risk quadrangle. The risk quadrangle provides a fundamental link between risk-averse optimization and statistical estimation. I will exploit this link to generate statistical models appropriate for risk-averse optimization. In addition, risk-averse quantities are often not differentiable in the classic sense. To make such quantities amenable to derivative-based optimization algorithms and global quadrature approximation, I will present a theory for smooth risk measures. I conclude my talk with numerical examples.

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Title: Multi-Scale Computational Homogenization of Microscale Localization Towards Macroscale X-FEM Description

Author(s): Varvara Kouznetsova, Emanuela Bosco, Marc Geers, *Eindhoven U. Tech.*.

In this talk a computational homogenization technique for the multi-scale modeling of material failure will be presented. Material failure is an intrinsically multi-scale process, which initiates at a fine microstructural scale and ultimately leads to macroscopic fracture. The proposed continuous-discontinuous computational homogenization-localization framework involves a discontinuity enhanced macroscale problem. In the previous work [1] the macroscopic discontinuity description relied on embedded discontinuities approach. The current contribution [2] presents a new formulation based on the partition of unity XFEM concept for the description of the macroscopic cohesive crack. The presented approach departs from classical computational homogenization. Upon the onset of strain localization, the microscale is characterized by a strain localization band (i.e. a band of high strains where damage grows) and by two adjacent unloading bulk regions at each side of the localization zone. To allow for the strain localization band development within the microstructural volume element (MVE) with minimal interference of the boundary conditions, percolation path aligned boundary conditions have been used, based on the projection of the boundary constraints onto the directions related to the developing localization band. The micro-scale localization band is lumped into a macroscopic cohesive crack, accommodated through discontinuity enriched macro-scale kinematics. Scale transitions [3] are formulated to retrieve two distinct bulk stress states at each side of the discontinuity, related by the continuity of the tractions at the interface, ensuring equilibrium. The effective displacement jump and the deformation discontinuity are derived from the micro-scale strain localization through a least square minimization of the true micro-fluctuation field. The governing response of the continuum with a discontinuity is obtained numerically in terms of cohesive crack traction-separation law and the stress-strain description of the continuous material at both sides of the discontinuity. The applicability of the developed computational homogenization framework has been demonstrated on representative benchmark problems involving the macroscale crack development as a result of the microstructural degradation. References [1]. Coenen E.W.C., Kouznetsova V.G., Geers M.G.D., A multi-scale approach to bridge microscale damage and macroscale failure: a nested computational homogenization-localization framework, Int. J. Fracture, 178, 157-178 (2012) [2]. E. Bosco, V.G. Kouznetsova, M.G.D. Geers, Multi-scale computational homogenization-localization for propagating discontinuities using X-FEM, Int. J. Numer. Meth. Engrg., (2015) [3]. E. Bosco, V.G. Kouznetsova, E.W.C. Coenen, M.G.D. Geers, A. Salvadori, A multiscale framework for localizing microstructures towards the onset of macroscopic discontinuity, Comp. Mech., 54, 299-319, (2014).

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Title: Automatic Hexahedral Meshing of Thin Regions Connected to Hex-Dominant Meshes

Author(s): Nicolas kowalski, Jean-François Remacle, Paul Emile Bernard, *U. Catholique de Louvain*.

The automatic generation of high quality hexahedral meshes is still an open and complex problem. At UCL, the team of Pr. Remacle provided recently an algorithm [Baudouin2014], available in Gmsh (free software) [Gmsh], to generate hex-dominant meshes for arbitrary geometries. This algorithm computes a frame field over the whole domain controlling the orientation of the obtained hexahedrals. Then, a frontal method based on the frame field fill the volume with vertices. A tetrahedral mesh is then generated using those vertices, and the obtained tetrahedra are merged into hexahedra, with some tetrahedra, prisms and pyramids remaining in some regions. However, in thin parts of the geometry, the quadrilateral surfacic meshes usually do not match, and surfacic vertices do not possess equivalents on the opposite surface. This leads to very low quality elements in those regions. We provide an algorithm that improves over the previous software of Pr. Remacle by: 1) Automatically recognizing the thin parts of the model and the two opposite surfaces, for which the distance from each other remains inferior to the desired mesh size 2) Assigning one of the two surfaces as master and the other as slave 3) Modifying the surfacic mesh of the slave surface to match the one of the master surface 4) Removing previous vertices that are now unnecessary Then, by running again the hex-dominant mesh generation algorithm, we are able to obtain a high-quality hex-dominant mesh for the whole volume, with structured full-hex meshes in the thin regions of the domain that are smoothly connected to the rest of the mesh. [Baudouin 2014] Baudouin, T. C., Remacle, J. F., Marchandise, E., Henrotte, F., & Geuzaine, C.(2014). A frontal approach to hex-dominant mesh generation. Advanced Modeling and Simulation in Engineering Sciences, 1(1), 1-30. [Gmsh] http://www.geuz.org/gmsh/

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Title: Kinetic and Potential Energy Analysis of Molecular Crystals with Emphasis on Chemical Decomposition of Solid Explosives

Author(s): Brent Kraczek, *US Army Rsch. Lab.*.

Molecular solids are used in a variety of applications, including pharmaceuticals, explosives, piezoelectrics and organic electronic components. In this talk we describe a novel approach to analyzing the thermal properties of molecular solids through an analysis of how the kinetic and potential energy in phonon modes is distributed within the individual molecules. This approach is based on quasiharmonic lattice dynamics (phonon) calculations. It captures both inter- and intra-molecular excitations with relevance thermal equilibrium and excited states and has particular relevance to studies of chemical decomposition. We apply our approach to the solid explosives aHMX and nitromethane. We explore how energy from impact and thermal loading transferred to phonon modes excite bonds important to chemical decomposition, with emphasis on the dynamics of the component molecules. A particularly important finding in HMX is that N-N bonds involved in the early stages of chemical decomposition are most strongly excited by low-frequency phonon modes, while no signal of this excitation is present in the kinetic energy analysis. These modes are typically ignored in investigations of chemical decomposition, as most experimental and computational techniques used to analyze the vibrational dynamics of the materials depend on relative atomic displacements. We conclude by discussing extensions of this analysis for use in other crystal engineering applications.

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Title: Probabilistic Assessment of Reinforced Concrete Structure Failure Under Extreme Temperature Using ANSYS Software

Author(s): Juraj Králik, *Slovak U. Tech.-Bratislava*; Peter Rosko, *Vienna U. Tech.*.

The paper presents an application of the nonlinear analysis of reinforced concrete structures under extreme static loads. The evaluation is based on an extension of the smeared rotated crack model developed on the basis of Chen bidimensional failure criterion and fracture energy provided by CEB-FIP Model Code 1990. The processes of the concrete cracking and crushing are developed during the increasing of the load. The concrete compres¬sive stress (fc), the concrete tensile stress (ft) and the shear modulus G are reduced after the crushing or cracking of the concrete. The layered approximation and the smeared crack model of the shell element are proposed. This nonlinear material model was adopted to the layered shell element (SHELL181) from the ANSYS library. The program CRACK under system ANSYS was verified in comparison with the experimental results on the reinforced concrete plate and wall. The inaccuracy of the structural model and resistance are determined by the quality of the considered model and numerical methods. The uncertainties of the loads level (dead, temperature and live loads), the material model (concrete cracking and crushing, behavior of the reinforcement), degradation effects and other influences following from the inaccuracy of the calculated model and numerical methods were taken into account in the response surface method (RSM). The RSM is the effective technique designed to find the best value of response considering the variability of the input data if these relations are continuous (not stepped). The coefficient of the approximation functions are determined by a second-order model using central composite design (CCD). The probability of the structure failure was considered using the Monte Carlo simulations and the criterion of the concrete failure. The program CRACK under system ANSYS was used for the analysis of the probability of failure of reinforced concrete structure of bubble tower under the extreme overpressure and temperature due to hard accident of technology. The calculation of the fragility curve to determine the failure pressure on the base of the nonlinear probabilistic analysis of the bubbler tower is presented.

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Title: Constrained Interpolation Remap for Interface-Capturing Finite Element Methods Applied to Multi-Material Electromagnetics

Author(s): Richard Kramer, Chris Siefert, Tom Voth, *Sandia Nat'l. Lab.*.

New conformal decomposition and extended finite element methods (CDFEM/XFEM) that capture material interfaces have recently been developed for electromagnetics problems. These present a compelling replacement for arbitrary mixture models in Arbitrary Lagrangian-Eulerian simulations, but demand a remap approach that is both compatible with the enriched mesh and can enforce zero divergence of the magnetic field. We present here a development of constrained interpolation (CI) remap [1] for both nodal and edge element discretizations for electromagnetics, applied to 2-D triangular CDFEM meshes. The concept of CI remap is elegantly simple: transfer a representation of a field that exists on a source mesh to a destination mesh such that a norm of interest is preserved (e.g., magnetic energy, the L2 norm of the B field). The destination field is formed from a convex combination of low and high order interpolations from the source mesh such that the norm is preserved element-wise as closely as possible. A local optimization problem seeks to minimize the difference between the norm of the source field on the elements of the destination mesh and the norm of the remapped field by choice of the parameter that blends the low and high order approximations. Results showing conservation and expected convergence rates are presented for the 2-D transverse electric form, where the magnetic field is node-based (Bz) and the preserved norm is the L2 of the nodal field; for the 2-D transverse magnetic form where a node-based vector potential of the magnetic field is remapped and the norm of its gradient, representing the magnetic energy, is preserved; and for the 2-D transverse magnetic form with an edge-based vector potential field, where the norm of the curl of the potential, i.e., the magnetic energy, is preserved. [1] Bochev, P. and Shashkov, M., Constrained interpolation (remap) of divergence-free fields, Comput. Methods Appl. Engrg. 194 (2005) 511-530. *Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

13th U.S. National Congress on Computational Mechanics
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Title: A Parallel and Monolithic Approach to FSI Combining Finite Elements and Finite Volumes

Author(s): Rolf Krause, Johannes Steiner, *U. Lugano*.

We present a monolithic approach for fluid structure interaction, which is based on the coupling of finite elements (solid) and finite volume (fluid). Here, the transfer of forces and displacements is fulfilled in a common set of equations for fluid and structure, which is solved simultaneously. We model the fluid by means of the incompressible Navier-Stokes equation , while we use a pure Lagrangian formulation for the structure. We discuss the coupling at the interface between the two discretizatios. We moreover discuss in detail the preconditioning of the arising systems and compare additive Schwarz and multigrid methods for the solution of the linear sub-problems in the arising Newton-steps. Finally, we present scaling results up to 2'000 cores for our parallel solution methods

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Title: Massively Parallel Strategies for Contact Problems - Interface Detection, Information Transfer, and Solution

Author(s): Rolf Krause, Patrick Zulian, *U. Lugano*.

The efficient solution of frictional contact problems in parallel puts high demands on the employed discretization and solution methods. On the side of the solution methods, parallel strategies have to be developed which are capable of dealing with the arising non-smooth energies. On the side of the discretization, also suitable strategies for the detection (and possibly the tracking) of the contact interfaces have to be developed. This is of particluar difficulty, as the identification of the contact interface in the case of meshes, which are arbitrarily distributed on different processors, requires communication between a priori unknown communication partners. This is particular difficulty for the widely used mortar method, as the mortar transfer operator at the interface can not be assembled in a straight-forward manner. In this talk, we first present a parallel decomposition approach for the solution of constrained smooth and non-smooth decomposition problems. In combination with a well designed multigrid method, our approach allows for the parallel solution of contact problems with optimal complexity. In the second part of our talk, we present a massively parallel strategy for the detection of possible contact interfaces, which is capable of dealing with arbitrarily distributed meshes. We also explain in what way projections (as, e.g. the L2-projection for the mortar-transfer operator) along interacting surfaces or between overlapping volumes can be efficiently realized in parallel.

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Title: Instance Optimality of the Adaptive Maximum Strategy

Author(s): Christian Kreuzer, *Ruhr U. Bochum*.

Adaptive finite element methods (AFEMs) for elliptic problems with the so called bulk chasing or Dörfler marking strategy converge with optimal rates provided the marking parameter is small enough. In contrast, numerical computations indicate that the maximum marking strategy is less sensitive to the choice of the marking parameter and in addition does not require sorting of the error indicators. In the model setting of Poisson's problem in 2d, we proof even instance optimality of an AFEM with a modified maximum strategy. This means that in each iteration the AFEM produces a quasi optimal total error with respect to the degrees of freedom (DOFs) up to a constant. Our approach is based on the minimisation of the Dirichlet energy and a newly developed tree structure of conforming triangulations created by newest vertex bisection.

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Title: A Stabilized Finite-Element Formulation for Diffusion in Incompressible Media Undergoing Large Deformations

Author(s): Andreas Krischok, Christian Linder, *Stanford U.*.

The numerical analysis of poromechanics models for hydrated materials with an almost or entirely incompressible matrix is still a major challenge for researchers. Standard mixed finite element formulations with an additional pressure degree of freedom are known to suffer from spurious pressure oscillations due to the violation of the inf-sup condition. Researchers have developed several stabilization schemes to cure these instabilities such as the very common but computationally less efficient use of quadratic basis functions for the displacements. In recent years, a lot of effort has been invested to develop stabilization schemes for equal order interpolations under the assumptions of small strains. The extension of these models to the finite deformation range, however, is still a topic of further investigation. Applications include the modeling of polymeric gels, biofilms, hydrated biological tissue or water-saturated soil undergoing elasto-plastic deformation. Recently, a first stabilized equal-order interpolation poromechanics model has been proposed in the finite deformation range [1]. In this work, a stabilization parameter is adaptively adjusted to avoid pressure oscillations and an F-Bar approach with an additional stabilization parameter is employed to cure volumetric locking in the incompressible limit. We investigate a classical approach to stabilize the pressure, based on an element-wise additional enhancement of the assumed strain field. The combined displacement/pressure/enhanced-strain discretization is known to exhibit hourglass patterns in the finite deformation range and has hence been abandoned as a possible inf-sup stabilization method [2]. We show that an alternative formulation of the local enhancement is free of hourglass patterns, fully inf-sup stable and capable to account for volumetric locking without the necessity to use additional parameters. The stability of the proposed formulation is investigated in swelling and indentation tests of polymeric gels with time-dependent diffusion as well as compression tests of rubber-like materials with an improved stress discretization. The proposed finite element discretization is applicable to material models which account for diffusion in an incompressible matrix undergoing large deformations and hence of particular interest for certain applications in Computational Geomechanics. [1] W. Sun, J.T. Ostien & A.G. Salinger, A stabilized assumed deformation gradient finite element formulation for strongly coupled poromechanical simulations at finite strain, International Journal for Numerical and Analytical Methods in Geomechanics, Vol. 37(16), 65-75, 2013. [2] D. Pantuso & K.J Bathe, On the stability of mixed finite elements in large strain analysis of incompressible solids, Finite Elements in Analysis and Design, Vol. 28, 83-104, 1997.

13th U.S. National Congress on Computational Mechanics
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Title: Work Heterogeneity Predicts Patient Response in Cardiac Resynchronization Therapy

Author(s): Adarsh Krishnamurthy, *Iowa State U.*; Christopher Villongco, Jeffrey Omens, Andrew McCulloch, *UC San Diego*.

Patient-specific image data combined with standard clinical measurements can be used to develop patient-specific computational models to compute regional cardiac function. Previous studies using animal and computational models suggested that increased heterogeneity in regional myocardial work density is a sensitive indicator of the mechanical deficit caused by electrical dyssynchrony in the failing heart. We therefore hypothesized that in dyssynchronous heart failure patients, functional improvements in response to Cardiac Resynchronization Therapy (CRT) may be greater in subjects with higher baseline heterogeneity of regional myocardial work. Three-dimensional bi-ventricular geometry was segmented from CT images of the heart at end-diastole. A finite-element ventricular model with 128 cubic-Hermite hexahedral elements was used to perform biomechanics simulations. Human myofiber and sheet architecture were computed from diffusion-tensor MRI obtained from an isolated, fixed human organ-donor heart and mapped to the patient-specific ventricular geometry using large-deformation diffeomorphic mapping. Passive myocardial properties were optimized while simultaneously computing the unloaded reference bi-ventricular geometry. Active myocardial contractile properties were optimized so that ventricular pressures measured by cardiac catheterization matched model predictions. Finally, a circulatory adaptation algorithm (CircAdapt) was used to estimate lumped-parameters of a closed-loop circulation model to match measured hemodynamic flow data. Simulation results for mechanical function were used to compute the distribution of the external work density in the left ventricle. These methods were applied in 8 heart failure patients who gave informed consent at the San Diego VA Medical Center. The methods were validated using echocardiographic measurements of regional wall motion that were not used as input to the model. Spatial distribution of myocardial work density computed from baseline models varied significantly between patients (mean 0.7-5.3, s.d. 1.0-6.5 kJ/m^3). Two measures of the distribution, LV fraction performing negative work and coefficient of variation (s.d./mean) correlated strongly with observed reduction in end-systolic volume after CRT (R^2=0.81, 0.79 respectively). In conclusion, functional improvement following CRT is greatest in patients with the largest region of LV performing negative work. REFERENCES Krishnamurthy et al. (2013) Patient-Specific Models of Cardiac Biomechanics. Journal of Computational Physics 244:4-21. Aguado-Sierra et al. (2011) Patient-Specific Modeling of Dyssynchronous Heart Failure: a Case Study. Progress in Biophysics and Molecular Biology 107(1). Kerckhoffs et al. (2010) Ventricular dilation and electrical dyssynchrony synergistically increase regional mechanical non-uniformity but not mechanical dyssynchrony. Circulation: Heart Failure 3:528-536.

13th U.S. National Congress on Computational Mechanics
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Title: HexJaal: A Bounded-Distortion Hex Mesh Generator Using Polycubes Method

Author(s): Chaman Singh Verma Krishnan Suresh, *U. Wisconsin*.

\begin{document} \maketitle An automatic, high quality hex mesh generation for arbitrary complex geometries is widely considered to be an open problem. Among many methods, {\em Polycubes} has many advantages including conceptual simplicity. However, its full automation poses many challenges. Our major contributions consists of following components in generating hex mesh using the Polycubes: \begin{enumerate} \item {\bf Distribution and placement of surface singularities:} Proper placement of singularities is critical in bounding the geometric qualities of a mesh. Since theoretical lower bounds (Guass-Bonnet theorem) on singular points may often produce mesh with large distortion, we use N-Rosy vector field \cite{keenan} as a directive to identify locations of singular points and incrementally place them on a given manifold to control the maximum distortion. \item {\bf A faster and reliable globally injective mapping:} We improve the methods of Lipman \cite{lipman}, and Sorkine \cite{sorkine} locally injective mappings to morph the model mesh into polycubes. Our method can handle very large meshes, provide global injectivity, produce elements with bounded distortion, fold-free, and fast enough for an interactive feedback. \item {\bf A selective dual sheet refinement:} The final step of our algorithm modifies the hexmesh using {\em selective sheets modification} approach. Our approach inserts dual sheets near the singular edges and only if it improves the geometrical qualities of the mesh. \end{enumerate} We have experimented with many free-form, and CAD models to generate hex-meshes. In the software pipeline, only the first component of mesh segmentation is semi-automated and time consuming, while all other components are fully automated and efficient. We developed a sketch based system to place the singularities on the model and were able to generate high quality hex mesh over complex domains. \bibliographystyle{ieeetr} \bibliography{polycubes} \end{document} @article{keenan, title={Globally optimal direction fields}, author={Kn{\"o}ppel, Felix and Crane, Keenan and Pinkall, Ulrich and Schr{\"o}der, Peter}, journal={ACM Transactions on Graphics (TOG)}, volume={32}, number={4}, pages={59}, year={2013}, publisher={ACM} } @article{lipman, author = {Aigerman, Noam and Lipman, Yaron}, title = {Injective and Bounded Distortion Mappings in 3D}, journal = {ACM Trans. Graph.}, issue_date = {July 2013}, volume = {32}, number = {4}, month = jul, year = {2013}, pages = {106:1--106:14} } @inproceedings{sorkine, author = {Sch\"{u}ller, Christian and Kavan, Ladislav and Panozzo, Daniele and Sorkine-Hornung, Olga}, title = {Locally Injective Mappings}, booktitle = {Proceedings of the Eleventh Eurographics/ACMSIGGRAPH Symposium on Geometry Processing}, series = {SGP '13}, year = {2013}, location = {Genova, Italy}, pages = {125--135}, numpages = {11} } ~

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Title: Mean-Deformation-Gradient 8-Node Hexahedron with Optimized Energy-Sampling Stabilization

Author(s): Petr Krysl, *UC San Diego*.

Ted Belytschko's lasting contributions to computational mechanics include the introduction of the mean-strain hexahedron technology. An important part of the development was stabilization of the element. In addition to the perturbation stabilization, Belytschko's group also developed the widely emulated assumed-strain stabilization. In the present contribution an alternative assumed-strain formulation with an alternative stabilization approach is developed. A method for stabilizing the mean-strain hexahedron for applications to anisotropic elasticity was described by Krysl (in IJNME 2014). The technique relied on a sampling of the stabilization energy using the mean-strain quadrature and the full Gaussian integration rule. This combination was shown to guarantee consistency and stability. The stabilization energy was expressed in terms of input parameters of the real material, and the value of the stabilization parameter was fixed in a quasi-optimal manner by linking the stabilization to the bending behavior of the hexahedral element (Krysl, submitted). Here the formulation is extended to large-strain hyperelasticity, for isotropic and anisotropic material models. The stabilization energy is expressed through a stored-energy function, and contact with input parameters in the small-strain regime is made. The stabilization parameter is again determined to optimize bending stiffness. The accuracy and convergence characteristics of the present formulations for both solid and thin-walled structures (shells) compare favorably with the capabilities of mean-strain, enhanced-strain, and other high-performance hexahedral elements described in the open literature. For thin structures the element is also competitive with successful shell elements. In summary -- The present formulation does not require an arbitrary stabilization parameter to be set by the user. -- The stabilization also works for arbitrarily anisotropic materials. -- Finally, the present stabilization improved coarse-mesh accuracy (bending) response to the point where the element is a contender in the analysis of thin-walled (shell) structures, while possessing excellent accuracy for solids. Hence the present formulation is believed to be a good general purpose tool for the large-strain analysis of solids and thin-walled structures. Acknowledgments Partial support from U.S. Navy CNO-N45, project management Frank Stone and Ernie Young, and continued support of Mike Weise (Office of Naval Research), is gratefully acknowledged.

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Title: Statistically Augmented Boundary Conditions (SABC) for Defining Statistically Equivalent RVE or SERVE's in Two-Phase Composite Materials

Author(s): Dhirendra Kubair, Somnath Ghosh, *Johns Hopkins U.*.

Statistically equivalent representative volume elements (SERVEs) are used to obtain homogenized constitutive responses of randomly dispersed two-phase composite systems [1,2]. The SERVE size is calculated iteratively, by systematically increasing the SERVE size, until the homogenized response saturates and becomes invariant with further increase in the SERVE size. Most computational homogenization techniques consider only the size of the SERVE in their description, while prescribing classical boundary conditions such as, affine-displacements, constant-stress or the periodic boundary-conditions. The classical boundary-conditions assume that the strain-energy-density is constant in the immediate vicinity of the simulated SERVE, which leads to overestimation the SERVE size. In the present study, we have derived novel boundary-conditions accounting for the microstructural description of the exterior domain using the modified Green's function approach. The randomly dispersed two-phase composite is quantified by 1- and 2-point correlation functions that describe the interactions between the fibers in the exterior. The modified boundary-conditions are superior compared to the classical boundary-conditions as they account for the microstructural details of the exterior and overcomes the truncation error of the integral-length-scale (the area under the 2-point correlation function). The novel boundary-conditions are very efficient even in the description of statistical volume elements (SVEs). With the classical boundary-conditions, the size of the SVEs required for convergence is larger than those subjected to the real boundary-conditions. The efficacy of the novel boundary-conditions is also exhibited in the definition of the weighted statistical volume elements (WSVEs). With the prescription of the real boundary-conditions, the homogenized modulus converges for all realizations of the WSVEs. A large number of realizations need to be considered for convergence of WSVEs with the prescription of the classical boundary-conditions. We have developed rate-independent and rate-dependent homogenized continuum-damage-model (HCDM) [2] that account for fiber disbonding and matrix damage along with inertia of the medium. References: [1] Swaminathan, S., Ghosh, S., and Pagano, N.J. (2006) Statistically equivalent representative volume elements for unidirectional composite microstructures: Part I-Without damage. Journal of Composite Materials, 40(7), 583-604. [2] Swaminathan, S., and Pagano, N.J. and Ghosh, S. (2006) Statistically equivalent representative volume elements for unidirectional composite microstructures: Part II-With interfacial debonding. Journal of Composite Materials, 40(7), 605-621.

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Title: Recent Advances in High-Order Discontinuous Galerkin Methods for Shallow Water Flow

Author(s): Ethan Kubatko, *Ohio State U.*.

In this talk, I will discuss some recent advances in the development and application of discontinuous Galerkin (DG) finite element methods for one-, two- and three-dimensional shallow water flow. Topics covered will include: (1) the development and implementation of a novel DG method that provides a unified approach for solving the two- (depth-integrated) and three-dimensional shallow water equations; (2) the use of H^1-conforming hierarchical shape functions in constructing the geometry of higher-order elements in support of this approach; and (3) the development of new efficient Lobatto-type numerical integration formulas for DG on simplexes and cubes.

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Title: The Living Heart Project: Modeling Pathologies of Systolic and Diastolic Heart Failure

Author(s): Martin Genet, *ETH Zurich*; LikChuan Lee, *Michigan State U.*; Brian Baillargeon, *Abaqus / Dassault Systemes*; Julius M Guccione, *UC San Francisco*; Ellen Kuhl, *Stanford U.*.

Chronic heart failure is a medical condition that involves structural and functional changes of the heart and a progressive reduction in cardiac output. Heart failure is classified into two categories: systolic heart failure, a dilation of the ventricles associated with reduced pump function; and diastolic heart failure, a thickening of the ventricular wall associated with impaired filling [1]. In theory, the pathophysiology of heart failure is well understood. In practice, however, heart failure is highly sensitive to cardiac microstructure, geometry, and loading. This makes it virtually impossible to predict the time line of heart failure for a diseased individual. Here we show that multiscale computational modeling allows us to integrate patient-specific knowledge from different scales to create an individualized model for cardiac growth and remodeling during chronic heart failure. Our model naturally connects molecular events of serial and parallel sarcomere deposition with cellular phenomena of sarcomerogenesis and myofibrillogenesis to whole organ function. We demonstrate that our Living Heart model can predict chronic alterations in chamber size, wall thickness, and cardiac geometry, which agree favorably with the clinical observations in patients with systolic and diastolic heart failure [2]. In contrast to existing single- or bi-ventricular models, our new four-chamber model can also predict characteristic secondary effects including papillary muscle dislocation, annular dilation, regurgitant flow, and outflow obstruction. Our prototype study suggests that computational modeling provides a patient-specific window into the progression of heart failure with a view towards personalized treatment planning [3]. [1] Göktepe S, Abilez OJ, Parker KK, Kuhl E. A multiscale model for eccentric and concentric cardiac growth through sarcomerogenesis. J Theor Bio, 2010;265:433-442. [2] Baillargeon B, Rebelo N, Fox DD, Taylor RL, Kuhl E. The Living Heart Project: A robust and integrative simulator for human heart function. Eur J Mech A/Solids. 2014;48:38-47. [3] Baillargeon B, Costa I, Leach JR, Lee LC, Genet M, Toutain A, Wenk JF, Rausch MK, Rebelo N, Acevedo-Bolton G, Kuhl E, Navia JL, Guccione JM. Human cardiac function simulator for the optimal design of a novel annuloplasty ring. Cardiovasc Eng Tech. doi:10.1007/s13239-015-0216-z.

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Title: Effect of Fibrillar Material on the In-Plane Strength and Stiffness of Paperboard

Author(s): Artem Kulachenko, Armin Halilovic, Hamid Reza Motamedian, *Royal Inst. Tech.*.

In-plane strength and stiffness of paper and packaging materials have always been among the top priorities for paper-makers. There are two traditional ways of improving paper strength with given raw materials and processes, namely, strength additives and mechanical refining of paper fibers (pulp). There is yet another alternative considered at the moment: adding cellulose nanofibrils (CNF). Both the refining and addition of CNF essentially introduce a fraction of fibrillar material, with dimensions significantly smaller (up to 1000 times) than the pulp fibers themselves. The exact mechanisms behind the strength improvement introduced by the fibrillar materials are still being discussed. They can potentially improve connectivity in the fiber network through increasing the number of bonds, but they can also reinforce the bond regions or redistribute the load between the fibers. In this work, we discuss the mechanism of strength improvement introduced by the addition of fibrillar material on the example of paperboard. We use micromechanical, fiber-level simulation tools, in which we resolve individual fibers, model contact between them as well as introduce the fibrillar material. The numerical finite-element model accounts for a number of nonlinearities, such as contact, debonding, plasticity on the fiber level and large strains and deflections. The results of numerical analysis, used in combination with traditional experimental methods and microCT imaging, show that the main effect from the fibrillar fraction comes through reinforcing the bond regions, making them both stiffer and stronger.

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Title: Tuning the Bulk Properties of Bi-Disperse Mixtures by Size Ratio

Author(s): Nishant kumar, Vanessa Magnanimo, Stefan Luding, *U. Twente*.

Granular materials are widely used as raw materials in various industries and several industrial processes often lead to the generation of granular systems with large size ratios [1]. It is known that the presence of fines influences the micro-mechanical behavior of granular systems [2]. However, to the best of our knowledge, no systematic study has been done to understand the effect of fines in a mixture, where the volume of fines is kept constant and only the size and hence the number of fine particles changes. The focus on this problem can be understood as in some industrial process, the fines can be expensive and we are interested in low cost versus high productivity. In this case, the problem must deal with finding the right (optimum) size of the fines to be substituted or added in smaller amounts. Further application can be the addition of stiffer additives to the base assembly to enhance the bulk modulus of the mixture. On the other hand, softer ingredients in the mixture could help to avoid fracture and improve material durability. Using Discrete Element Method (DEM), we conclude that when a small number of additional particles with a similar size as that of the base assembly will barely affect the bulk modulus of the original assembly. On the other hand, when the number of fine particles is very large (much smaller radius), most of them will lie in the voids of the base material, and will act as rattlers [1], leading to no positive contribution to the bulk system. There is an optimum number (size) of particles to be added to the base material that maximizes (non-monotonously) the bulk modulus and other macroscopic quantities, and depends on the operating volume fraction. We show that the effective (bulk) stiffness of an ideal monodisperse assembly can be enhanced (or decreased) up to 20% by substituting as little as 5% of its volume with smaller particles of suitable size. Other properties and different volume ratio of fines are subject of present research. REFERENCES [1] Nishant Kumar, Olukayode I. Imole, Vanessa Magnanimo, and Stefan Luding. Effects of polydispersity on the micro-macro behavior of granular assemblies under different deformation paths. Particuology, 12:64–79, 2014. [2] N. Kumar, S. Luding, and V. Magnanimo. Macroscopic model with anisotropy based on micro-macro information. Acta Mechanica, 225(8):2319–2343, 2014.

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Title: Underwater Collapse of Tall Granular Columns

Author(s): Krishna Kumar, Kenichi Soga, *U. Cambridge*; Jean-Yves Delenne, *U. Montpellier Supagro*.

Geophysical hazards usually involve multiphase flow of dense granular solids and water. Understanding the mechanics of granular flow is of particular importance in predicting the run-out behaviour of submarine landslides. The collapse of a vertical cliff underwater results in complex momentum transfer between the solid phase and the fluid phase. Hence, it is important to understand the mechanism of underwater granular flows at the grain scale. In this study, two-dimensional sub-grain scale numerical simulations are performed to understand the local rheology of dense granular flows in fluid. The Discrete Element (DEM) technique is coupled with the Lattice Boltzmann Multiple-Relaxation-Time Method (LBM-MRT), for fluid-grain interactions, to understand the evolution of immersed granular flows. GPGPUs are used to simulate millions of LBM nodes. In contrast to short columns, the amount of material destabilised above the failure plane is larger in the case of tall columns and hence, the surface area of the mobilised mass that interacts with the surrounding fluid is significantly higher. This increase in the area of soil - fluid interaction results in an increase in the formation of turbulent vortices that alter the deposit morphology during the collapse. The distribution of mass in a granular flow plays a crucial role in the flow kinematics. The collapse of tall columns under different slope angles are studied. The collapse of a granular column in fluid involves three stages. The initial stage is characterised by the free-fall of grains above the failure surface. In this stage, the soil grains experience drag forces during free-fall resulting in a significant drop in the kinetic energy available for the flow. As the grains reach the static region, they collide with the neighbouring grains and are pushed away from the static cone. The kinetic energy gained during the free fall is converted into horizontal acceleration at this stage. The interactions between the soil grains on the flow surface with the surrounding fluid result in the formation of eddies, which is unique to this stage. The number of eddies formed during the flow is proportional to the surface area of the granular mass interacting with the fluid. Hydroplaning is observed at the flow front. The final stage involves dissipation of excess pore-pressure in the system and sedimentation and deposition of grains. The vortices interact with the granular mass and result in formation of heaps that significantly affect the distribution of mass in the flow. This behaviour is distinct from that observed in the case of short columns. A parametric analysis is performed to assess the influence of the granular characteristics (initial packing, permeability, slope of the inclined plane) on the flow kinematics of collapse of tall columns in fluid.

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Title: A Quasi-Harmonic-Based, Multi-Scale Method to Model Intrinsic Dissipation in Solids

Author(s): Kumar Kunal, Narayana Aluru, *U. Illinois, Urbana-Champaign*.

The high frequency vibrations in nano-electro mechanical systems (NEMS) have a number of important practical applications. The potential use of NEMS for all these applications is limited by damping. For vibrations in the GHz regime, the time-scale of mechanical deformation becomes comparable to the local equilibration time. This leads to an additional dissipation known as the Akhiezer damping(1). The condition of local equilibrium, as is often used in the existing quasi-harmonic methods(2) (QHM), remains no longer valid. In this work we extend the quasi-harmonic frame-work to model the intrinsic dissipation in solids under such high frequency vibrations. In the proposed frame-work we introduce a non-equilibrium component of the stress tensor that captures the interaction between the mechanical deformation and the thermal vibrations or phonons. The stress component characterizes the deviation from local equilibrium and vanishes under quasi-static deformation. A constitutive relation that governs the time evolution of the non-equilibrium stress is obtained. The relaxation rate for the stress tensor is obtained using Langevin dynamics in the space of normal modes. In this approach, each of the modes is modelled as a noisy harmonic oscillator. The other parameters for the constitutive relation are obtained using QHM. We, then, use this method to study the effect of surface on the Q factor, a measure of the inverse of damping rate. Vibrations with frequency in the range of few GHz are considered. The results are compared with those obtained using molecular dynamics simulation. References: 1) K. Kunal and N. R. Aluru, ``Akhiezer damping in nanostructures'', Physical Review B, Vol. 84, No. 24, Art. No. 245450, 2011. 2) Z. Tang, H. Zhao, G. Li and N. R. Aluru, ``Finite-temperature quasicontinuum method for multi-scale analysis of silicon nanostructures'', Physical Review B, Vol. 74, No. 6, Art. No. 064110, 2006.

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Title: Application of a Discrete Vortex Method to Analyze the Vortex Flow Induced by an Oscillating Flat Plate

Author(s): Yusuke Kunii, *Keio U.*.

In the field of micro air vehicle, introduction of the flapping-wing flight is awaited because of its energy efficiency and high maneuverability(1). However, not much is known about the mechanism of flapping flight as compared to those of rotors, and its comprehension requires both experimental and numerical approaches. The numerical approach to the flapping flight requires the treatment of moving boundaries. Thin boundary layer separating from the edge requires a high spatial resolution around the body. It is also required to cover a large computation domain, hence numerous numbers of discrete points are needed when a grid-based Eulerian methods such as finite volume or finite element methods are adopted. The vortex method is suitable for numerical analysis on the flapping flight because of its mesh-less nature and capability of treating deformable, moving boundaries. However, the vortex method is still under development and some issues needs to be addressed before it is used to practical applications. The precise treatment of the wall boundary is one of unresolved problems. The objective of this study is to apply a vortex method to the flapping flight analysis and to acquire knowledge on the relation between vortex flow structure and force induced by flapping flight. Firstly, to ensure the validity of calculation code, the assessment of a numerical method for vortex method has been performed in the flow caused by an impulsively starting circular cylinder. Secondly, to verify our scheme, the code has been applied flow around an oscillating flat plate at a constant frequency and amplitude, which represents the fundamental model of flapping flight. The results on temporal development of the drag force of the cylinder agreed well with the analytical solution(2) and reference data(3), whereby the consistency and converging behavior of the scheme are confirmed as well. The force exerted on the plate by the oscillating plate was found to be plausible, in terms of the frequency and the phase-lag between the force and plate motion, despite some scattering in the data. (1) Ansari, S. A. et al. (2006), Prog. Aerosp. Sci., vol. 42, pp. 129-172 (2) Bar-Lev, M. and Yang , H. T. (1975), J. Fluid Mech., vol. 72, part 4, pp. 625-647 (3) Ploumhans, P.and Winckelmans, G. S. (2000), J. Comput. Phys., vol. 165, pp. 354-406

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Multi-Scale Analysis of Electrical Contact Resistance for Resistance Spot Welding Simulation

Author(s): Hiroyuki Kuramae, *Osaka Inst. Tech.*; Riku Kusumoto, Junya Yamada, Tomoya Niho, Tomoyoshi Horie, *Kyushu Inst. Tech.*.

Since electrical contact resistance is an important property in the numerical simulations for resistance spot welding, a multiscale coupled finite element (FE) procedure for resistance spot welding is developed to evaluate high accuracy of electrical contact resistance. The multiscale analysis consists of macroscopic FE analysis for resistance spot welding and microscopic electrical contact resistance analysis using three-dimensional thermal elasto-plasticity contact FE simulation. The multiscale analysis is based on coupled FE procedure among structural deformation, electric current and temperature to evaluate nugget growth by Joule heating in the macro-scale, and to calculate the electrical contact resistance in the micro-scale. Temperature-dependent material properties such as yield stress, work hardening rate and resistivity are considered in both scale analyses. A micro-FE model, which corresponds to statistically similar representative volume element (SSRVE), was constructed based on surface roughness measurement of a steel sheet using laser microscope apparatus. In this study, the size of SSRVE in-plane was determined and sampled as 40×40μm2 by comparing the frequency distribution of surface roughness from measured area 1411×1058μm2 with 0.689μm interval. A rigid plate is contacted to the micro-FE model with contact pressure and temperature that are obtained by macro-analysis, to calculate electrical contact resistance. The micro-FE analysis was conducted by an elast-plasticity contact FE code including large deformation theory combined with electric FE code based on the φ-method to compute the electrical contact resistance of deformed shape of SSRVE every time step. A micro-FE analysis is assigned to each of contact FEs on the macro-FE mesh between steel sheets to obtain electrical contact resistance. In order to investigate the multiscale FE result, a conventional single-scale FE analysis which is only macroscopic resistance spot welding FE analysis using the Bubu's model [1] to evaluate the electrical contact resistance was also performed and compared with the multiscale FE result. It was confirmed that the nonlinear effects of time history of electrical contact resistance by loading paths of contact pressure and temperature. As a result, temperature of multiscale analysis was lower than that of single-scale one, because electrical contact resistance by the Babu's model was higher than the multi-scale FE result. References: [1] S.S. Babu, M.L. Santella, Z. Feng, B.W. Riemer and J.W. Cohron, Empirical model of effects of pressure and temperature on electrical contact resistance of metals, Sci. Tech. Welding Joining, Vol. 6-3, pp. 126-132, 2001.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: A Method for Fracture Simulation of Concrete Using an Isotropic Damage Model

Author(s): Mao Kurumatani, Shunitsu Abe, Yuki Nemoto, Yuto Soma, Norikazu Henmi, *Ibaraki U.*.

Concrete materials are highly heterogeneous and inhomogeneous in meso- or micro-level spatial scale, which causes the quasi-brittle fracture with multiple and complex cracking. The numerical simulation of the propagating cracks in concrete is an important task in civil and computational engineering. In order to realize the failure simulation of concrete or reinforced concrete, it is necessary to develop a method which is capable of robustly representing the fracture behavior with multiple cracking. In this study we present a method for simulating fracture behavior in concrete involving multiple cracking. The cracks are modeled as the degradation of material stiffness, that is to say, treated as the material damage for robustly representing multiple cracking. The damage model applied in this study is based on fracture mechanics for concrete, and is capable of analyzing quasi-brittle fracture with the fracture energy. For simplicity and robustness, it is assumed to be isotropic. The isotropic damage model is incorporated into the finite element method. First, the isotropic damage model is formulated, and the basic performance of the damage model is verified in several numerical experiments. Then we simulate 3-D crack propagations in concrete. The internal cracks formed in concrete around deformed bars and the fracture behavior of RC beams are simulated by using the suggested method with the damage model. It is shown that the results obtained by the numerical analyses with the damage model are conformable with that presented in the literature.

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Title: A Generalized Continuum-Based Homogenization Model for 3D Woven Material

Author(s): Sergey Kuznetsov, *N. I. Lobachevsky State U.*; Boris Fedulov, *Skolkovo Inst. Sci. & Tech.*; James Guest, *JHU*.

Computational homogenization became an important tool in computational materials science. A lot of work still has to be done to make it a reliable and versatile tool for industrial applications. In particular, the range of applicability has to be extended and computational efficiency has to be improved[1]. For many heterogeneous materials, in particular, some composites, porous materials, there is experimental evidence of dependence of macroscopic material properties on the type of loading or type of deformation, since behavior of micro-constituents significantly depends on the character of external exposure: there might be differences in moduli for tension and compression, shear-tension interaction e.t.c. [2]. For example, in fabric-based composites and porous materials, the fibers are tightened up under tension but can bend and buckle into the pores space under compression. The differences in the mechanism of deformations provide dependence of the macroscopic properties on the loading conditions. Due to the differences in the bending and tensile stiffnesses, the elastic modulus of the composite under tension can be greater by a factor of 4 or 5 then the elastic modulus under compression[3]. Classical approaches do not allow to describe deformation of such media due to the absence of unified stress-strain dependencies. Nonlinear homogenization is capable to obtain numerical stress-strain dependencies, but these are implicit and local, therefore don’t let characterize stress-strain relation in the whole; this would require infinite number of calculations. There are reduced order nonlinear homogenization approaches attempting to estimate material behavior in the whole[1]. We use an alternative approach by assuming a specific generalized constitutive material behavior, characterized by material functions depending on a stress state parameter[2], and apply homogenization approach to obtain these material functions. The RVE is subjected to a number of complex multi-axial overall deformations, which allows to determine material functions. A variant of periodic boundary conditions, allowing complex macroscopic deformation and constraining microscopic fluctuations to be periodic are used. References 1. J. Fish, Practical Multiscaling, Wiley (2013)s 2. Lomakin, E.V.: Mechanics of media with stress-state dependent properties. Physical Mesomechanics. 10(5), 41-52 (2007) 3. Kratsch, K. M., et al, Carbon-carbon 3-D ortohogonal material behavior. AIAA Paper, 365 (1972)

13th U.S. National Congress on Computational Mechanics
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Title: Non-Linear Localized Deformation Waves in the Continuum with Internal Oscillatory Degrees of Freedom

Author(s): Sergey Kuznetsov, *NUST MISIS; Johns Hopkins U.*; Vladimir Erofeev, *Mech'l. Eng. Rsch. Inst. RAS*.

Materials with microstructure with high contrast in mass, stiffness, isolated and interconnected structural element such as in 3d woven materials demonstrate a number of complex phenomena under external excitations, including formation and interaction of localized waves, transfer of energy from macroscopic oscillations to microscopic, energy dissipation, internal resonances e.t.c. Such diversity is related to the dynamical processes occurring at the microscopic level. It is very important to be able to model such phenomena for practical applications. At same time it is an extremely complex task due to coupling between spatial and temporal scales and need to introduce very high spatial and temporal resolution. An alternative approach is to consider an effective media with internal degrees of freedom. The existence of a carrying media is postulated and it is assumed that this media is described by equations on nonlinear elasticity theory. It is further assumed that infinite number of non-interacting oscillators is coupled with each point of the carrying medias[1]. It is shown that for one-dimensional wave processes the system of dynamics equations of generalized continuum is equivalent to the Korteweg-de Vries-Burgers equation. This equation has an analytical solution in the form of a spatially-localized wave. The influence of such parameters as stiffness, viscosity, and ratio of carrying media density to the oscillators' density on the magnitude, wave speed and the thickness of an impulse-like wave is studied. A non-stationary process of deformation wave localization is studied numerically. References 1. V. A. Palmov, Application of a Generalized Continuum Theory to the Problem of Spatial Damping in Complex Mechanical Systems, Computational Continuum Mechanics (2009), Vol. 2(4), pp. 105-110

13th U.S. National Congress on Computational Mechanics
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Title: A Posteriori Error Estimation Based on a Serendipity Pairing of Approximation Spaces in Isogeometric Methods

Author(s): Trond Kvamsdal, Mukesh Kumar, Kjetil A. Johannessen, *NTNU*.

There is at the moment a rapid progress within the IGA community regarding local refinable splines. We have in our group been working with LR B-splines, see references [1-3]. In [1] we pioneered the use of LR B-splines for adaptive IGA, and in [2] we developed superconvergent patch recovery techniques suited for LR B-splines, whereas in [3] we construct an error estimator based on a Serendipity pairing of approximation spaces that we will present herein. The idea of a Serendipity pairing of discrete approximation spaces Shp,k - Shp+1,k+1 where the space Shp+1,k+1 is considered as an enrichment of the original basis of Shp,k by means of the k-refinement, utilizes a typical unique feature available in isogeometric analysis. The space Shp+1,k+1 is used to obtain a higher order accurate isogeometric finite element approximation and using this approximation we propose two simple a posteriori error estimators. The proposed a posteriori error based adaptive h-refinement methodology using LR B-splines are tested on classical elliptic benchmark problems. The numerical tests illustrate the optimal convergence rates obtained for the unknown, as well as the effectiveness of the proposed error estimators. [1] K. A. Johannessen, T. Kvamsdal and T. Dokken: Isogeometric analysis using LR B-splines, Computer Methods in Applied Mechanics and Engineering, 269(2014), 471-514. [2] M. Kumar, T. Kvamsdal, and K.A. Johannessen: Superconvergent patch recovery and a posteriori error estimation technique in adaptive isogeometric analysis. Submitted to Computer methods in applied mechanics and engineering, 2014. [3] M. Kumar, T. Kvamsdal, and K.A. Johannessen: A simple a posteriori error estimatior in adaptive isogeometric analysis. Accepted by Computer and Mathematics with Applications, 2015.

13th U.S. National Congress on Computational Mechanics
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Title: Coupled Modeling of Non-Newtonian Blood Flows Through Distensible Viscoelastic Arteries

Author(s): JaeHyuk Kwack, Arif Masud, *U. Illinois, Urbana-Champaign*.

We present a stabilized mixed finite element method for fluid-structure interaction incorporating incompressible non-Newtonian fluids through viscoelastic arteries. The fluids and solids are coupled monolithically and a simultaneous solution procedure is employed. The momentum-balance equations for the solid domain are written in the Lagrangian description, and the equations for the incompressible non-Newtonian fluids are written in the Arbitrary Lagrangian Eulerian (ALE) description to account for finite deformation of the domain boundaries. We employ the Variational Multiscale (VMS) ideas to derive a stabilized fluid-solid interaction formulation. This formulation successfully addresses some of the most challenging stability issues, namely, the Babuška-Brezzi inf-sup condition that arises in mixed form of governing equations, and high convective effects at high Reynolds number flows. Benchmark problems are presented for verification of the method. Representative patient-specific blood-artery interaction simulations are presented.

13th U.S. National Congress on Computational Mechanics
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Title: Evolution of Anisotropy in Ductile Fracture Models

Author(s): Soondo Kweon, *Southern Illinois U.*.

Most metals get to possess induced anisotropy due to plastic deformation that produces texture, i.e., anisotropy, in manufacturing processes. Metals used in aerospace/nuclear applications are highly anisotropic regardless of their manufacturing processes. The effect of anisotropy plays a significant role in the ductile fracture process of metals as many experimental evidences indicate the correlation between texture and fracture. Fracture in ductile metals occurs after a large strain through which the anisotropy direction and strength change. However, ductile fracture models thus far have not been able to take into account the evolution of anisotropy adequately; the Hill parameter that are used to describe the plastic anisotropy and the direction of the orthotropy bases have been assumed to remain unchanging through large deformation until fracture is reached in ductile fracture models. Therefore, this study employs a recently proposed anisotropic ductile fracture model [1] that takes into account the evolution of anisotropy. In the proposed model, the evolution of the orthotropic bases is described using the plastic spin tensor, which is based upon the mechanics of the slip process. Shear damage has been observed in many experiments although it is not well understood theoretically why damage occurs in shear deformations where stress triaxiality is assumed to be zero. To reveal the source of damage in shear, this study simulated shear simulations of anisotropic metals with a RVE (Representative Volume Element) that has a void in the center. The evolution of the orthotropic bases is taken into account to accurately model anisotropy evolution in the shear simulation. The simulation result indicates that stress triaxiality can become as large in shear deformations as in uniaxial tension due to anisotropy and its evolution in shear deformations. The current theory of anisotropy evolution is in its primitive stage and it does not accurately capture the trend of anisotropy evolution shown in experiments. The theory of anisotropy evolution can be derived by crystal plasticity simulations. Therefore, this study investigates anisotropy evolution in FCC and BCC metals using texture analysis and crystal plasticity simulations. These simulation results will provide the basis for the theory of anisotropy evolution in the macro scale. References [1] S. Kweon. Investigation of shear damage considering the evolution of anisotropy. Journal of the Mechanics and Physics of Solids, 61, 2605–2624, 2013.

13th U.S. National Congress on Computational Mechanics
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Title: On the Effectiveness of Buried Elastic Bodies as Passive Vibration Isolators for Foundations Interacting with the Soil

Author(s): Josue Labaki, Euclides Mesquita, *U. Campinas*.

The present article introduces a model of the inertial response of two elastic bodies interacting with each other and with their surrounding soil. The soil is modeled as a viscoelastic, transversely isotropic, three-dimensional half-space. The boundary-value problem corresponding to the case of time-harmonic distributed axisymmetric vertical ring loads within a half-space is formulated. Its solution results in the required influence functions for the modeling of the present problem. Each of the elastic foundations is modeled as a thin circular plate with mass. The plate representing the foundation rests at the surface of the half-space and a buried plate represents the passive vibration isolator. The deflection profile of each plate is written in terms of generalized coordinates. The strain energy of the plates is written in terms of these generalized coordinates. The inertia of the plates is properly taken into account in this model by considering also the kinetic energy of each plate. The strain energy of the system involving the two plates and the half-space is obtained; it contains a parcel from each plate individually as well as the coupled interaction they have with each other. The generalized coordinates are determined by the solution of the Lagrange's equation of motion, which involves the strain and kinetic energy of the plates and of their surrounding medium, as well as the potential energy due to the external loads. A set of Lagrange multipliers is incorporated into the equation of motion so that the boundary conditions at the edge of the plates are satisfied. The solution of the constrained Lagrangian function results in the deflection profile of the plates. The paper investigates the effect of construction parameters of the embedded plate in the vibratory response of the foundation. These parameters include the stiffness and mass of the plates, the depth of embedment, outer radii and constitutive properties of the soil. The present numerical scheme contributes to the understanding of techniques to cope with the strict vibration requirements of sensitive structures, such as synchrotron light sources and nanoscience facilities.

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Title: Verification of Reduced-Order Modelling Codes with Truncated Bases

Author(s): Nicholas LaBarbera, *Penn. State U.*; Jonathan Pitt, *Penn. State U.* .

In recent years, simulations have become an increasingly important part of the engineering design process. This has caused a demand for the ability to compute solutions that are both accurate and computationally affordable. High-accuracy simulations often consist of linear systems with millions of degrees-of-freedom numbering in the millions, such as a high-fidelity simulation of the flow in a turbine engine. Running high-fidelity simulations can form a bottleneck in the design process. Reduced-order models derived from high-fidelity simulations offer a way to alleviate the bottleneck. One reduced order modeling technique is to use snap-shots from a high-fidelity simulations to derive a reduced order basis, which is significantly smaller then the basis used in the high-fidelity simulation. The governing equations are then projected onto the reduced order subspace. By working in a much lower dimensional subspace, significant computational savings are reaped. This work employs the Proper Orthogonal Decomposition (POD) method to obtain a set of basis functions for the reduced order model, which are then used as the basis vectors for the finite element method based discretization of the differential equations. With either a full-order or a reduced- order model, it is important to verify that the discrete equations were correctly implemented into a computer code. There are well developed techniques for rigorously verifying full-order models, such as the method of manufactured solutions; however, this technique cannot be applied to reduced-order models with an incomplete basis because the error might not converge to zero for an arbitrary exact solution. To address the problem, we present a method for verifying reduced-order models of truncated bases, using a modified method of manufactured solutions approach. In particular, we demonstrate that careful selection of an exact solution in the span of the reduced order model truncated basis results in proper convergence of the approach. To the best of the author's knowledge, there is no published verification strategy to confirm the correct implementation of a combined POD/Galerkin method.

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Title: Peridynamic Modeling of Different Severe Plastic Deformation Processes

Author(s): Gábor Ladányi, *College Dunaujvaros*.

Severe plastic deformation techniques are a dynamically researched way of advancing mechanical properties of materials via grain refinement. Common property of these techniques is the large plastic – primarily shear strain – deformation [1]. Modeling the severe plastic deformation with finite element method is complicated because of the high distortion of elements. Using remeshing techniques the problem can be avoided but the traceability of the results become difficult and accuracy usually decreases. In our presentation short introduction is about our applications of some SPD techniques to refine grain size in different metals (OFHC Cu, Al1050 and ARMCO Pure Iron). Available analytical and numerical models are also shown briefly with their results and capabilities. Peridynamic material model is well known as appropriate model to describe crack initiation and propagation in one hand without the necessity of special crack tip kinetics. In the first years most of the applications concentrated to brittle fracture. Recently, other possible fields – plasticity, thermo-elasticity, visco-elasticity, etc – of applications are introduced in several publications. After combining finite element models with peridynamic segments of bodies, nowadays the combination of meshless methods (Smooth Particle Hydrodynamics, Reproducing Kernel Particles Method, Radial Basis Functions) and peridynamics seems to be very fruitful. We applied the RKPM in state-based peridynamics as it was suggested in [2] to model different – mentioned above – SPD techniques. Application of peridynamics and RKPM – because they are meshless methods – do not suffer from the disadvantages of distorted element and time-consuming remeshing. On the pressure of SPD processes the applicability of usual Culomb's friction model is limited. Approved friction models are necessary. In our presentation we demonstrate friction modelling in peridynamic context with short discussion of experiences and effect on SPD results. The comparing of experimental, FEM and peridynamic result of SPD processes are also included. [1] B. Altan - Severe Plastic Deformation: Towards Bulk Production of Nanostructured Materials, 2005, New York, Nove Science Publisher Inc., ISBN 1-59454-508-1 [2] M. A. Bessa, J. T. Foster, T. Belytschko, Wing Kam Liu - A meshfree unification: reproducing kernel peridynamics, Computational Mechanics , June 2014, Volume 53, Issue 6, pp 1251-1264

13th U.S. National Congress on Computational Mechanics
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Title: Verification and Effectivity of PGD Computational Techniques

Author(s): Pierre Ladeveze, David Neron, *ENS Cachan*; Pierre-Eric Allier, Ludovic Chamoin, *LMT Cachan*.

Mechanics, like other domains, continues to supply numerous engineering problems that, despite the impressive progress of computational simulation techniques, remain intractable today. RB, POD and PGD model reduction methods are leading to a new generation of high-performance computational tools which provide solutions to engineering problems which are inaccessible to standard codes based on classical and well-established numerical techniques. This is a true breakthrough with a potential gain of several orders of magnitude. The approach we are considering here is the Proper Generalized Decomposition (PGD) which can be seen as an extension of POD. The main idea consists in calculating the shape functions and the solution itself simultaneously offline using an iterative procedure. A priori, these shape functions are arbitrary and must satisfy only a variable separation hypothesis, this hypothesis being also at the center of POD and RB reduction methods. The first part of the lecture deals with the different techniques for the computation of PGD approximation. They include the new one [4] , based on the “PGD-error indicator” introduced in [2,3]. For that, we use a benchmark proposed by S. Idelshon which is a unidimensional transient thermal problem with a moving load, the parameter being the velocity of the load . The reference to quantify the effectivity is the H1-SVD of the “exact” solution. Error estimators are also computed and their efficiency analysed. The end of the lecture is to examine the validity of the variable separation hypothesis, which is central in the PGD. Non-separated shape functions are also studied. REFERENCES [1] P. Ladevèze. Nonlinear Computationnal Structural Mechanics—New Approaches and Non-Incremental Methods of Calculation. Springer Verlag (1999). [2] P. Ladevèze, L. Chamoin. On the verification of model reduction methods based on the Proper Generalized Decomposition. Computer Methods in Applied Mechanics and Engineering, 200: 2032-2047 (2011). [3] P. Ladevèze, L. Chamoin. Towards guaranteed PGD-reduced model, Editors G. Zavarise and D.P. Boso. Publisher CIMNE, Bytes and Science 292 (2012). [4] P.E.Allier , L. Chamoin and P.Ladevèze, Proper Generalized Decomposition computational methods on a benchmark problem , AMSES , Springer [5] F. Chinesta, P. Ladevèze. Separated Representation and PGD-Based Reduction, Course CISM 554, Springer (2014).

13th U.S. National Congress on Computational Mechanics
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Title: Stabilized Finite Element Methods for Carbon Sequestration Modeling

Author(s): Chris Ladubec, Robert Gracie, *U. Waterloo*.

The reduction of CO2 emissions has been identified as a means to reduce global warming. CO2 emissions can be diverted and permanently stored in deep saline aquifers, which contain a resident brine solution. This process is known as carbon sequestration. Numerical modeling of carbon sequestration requires stochastic methods to address a tremendous amount of uncertainty in these systems. Stochastic methods require computationally efficient numerical models for site assessment simulations to be tractable. We have developed efficient models based on vertically averaged mass balance equations for CO2 and the resident brine. To the authors' knowledge our work, which includes [1], is the first study of the vertically averaged multiphase flow equations [2] in the finite element framework. Two coupled partial differential equations are solved that govern the evolution of brine and CO2 in a porous medium. A pressure equation describes the pressure in the system and a saturation equation models the evolution of the CO2 distribution. The saturation equation contains an advection operator. The Galerkin Finite Element Method (FEM) can produce nonphysical oscillations when solving this equation. We present and compare several alternative FEM formulations to reduce/remove the oscillations and improve stability of the simulations - the Streamline Upwind method (SU), the Streamline Upwind Petrov Galerkin method (SUPG) and the Least Squares Finite Element Method (LSFEM). Several examples demonstrate and compare the four spatial discretization approaches of the hyperbolic saturation equation. References 1. Ladubec, C., Gracie, R. and Craig, J. (2014). An extended finite element method model for carbon sequestration . Int. J. Numer. Meth. Engng., doi: 10.1002/nme.4737 2. Celia, M. A., & Nordbotten, J. M. (2009). Practical modeling approaches for geological storage of carbon dioxide. Ground Water, 47(5), 627-638.

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Title: Extending Spatial Simulation Domains of Existing Applications with Minimal Invasiveness

Author(s): Michael Lahnert, Miriam Mehl, *U. Stuttgart*.

Dynamically-adaptive, tree-structured cartesian grids are a well-known way of solving partial differential equations with less computational effort than regular cartesian grids and lower memory requirements than unstructured grids. However, adaptivity complicates accessing specific grid regions and makes it necessary to either traverse the entire grid or use search algorithms. Moreover, the information obtained by search algorithms needs to be updated whenever cells are dynamically refined and coarsened during the simulation. For this reason, there are many simulation codes that use regular grids to discretize the spatial domain. Ordering cells is an easy way to traverse a grid without visiting the same cell multiple times. For tree-structured cartesian grids, space-filling curves provide a way to order cells globally. At the same time they keep changes in cell ordering local if we adapt the grid by refining or coarsening cells. Although there are many implementations of dynamically-adaptive cartesian grids based on this idea, most of them traverse the grid only in this very specific way. This ensures great data locality. However one loses almost all flexibility in the way data is stored and accessed. To make adaptivity more accessible, we introduce a new concept for dynamically-adaptive cartesian grids based on Morton-ordering of cells and nodes. This framework permits transparent adaptivity by using an iterator-based approach for both data in cell-centers and data on cell-edges. This iterator-based approach allows traversing the grid in other ways than following along the space filling curve. Our algorithms allow for identifying cells, locating them in the grid, searching a cells' neighbors, and mapping nodal data to their corresponding cells. Our framework allows us to use a two-step process to integrate spatial adaptivity into an existing application that uses regular grids. First, we adapt the algorithms to cope with the additional numerical issues imposed by spatially-adaptive cartesian grids, such as hanging nodes located on refinement boundaries. Second, we optimize the data structures and data access patterns in order to maximize the benefits that space-filling curves provide due to good data locality. Using simple applications, we show potential savings compared to regular grids in terms of computational cost and storage. Besides, we investigate cache usage and runtime per unknown. Moreover, we demonstrate the ease of integrating our API in existing codes.

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Title: Rhino 3D to Abaqus Design-Through-Analysis: T-spline Based Isogeometric Analysis Software Solution

Author(s): Yicong Lai, Joshua Chen, Lei Liu, Yongjie Jessica Zhang, *Carnegie Mellon U.*; Eugene Fang, Jim Lua, *Global Engineering & Materials, Inc.*.

Abstract: This talk presents a novel software solution for T-spline based isogeometric analysis (IGA) in a fully-encapsulated environment for engineering design-through-analysis. Although T-spline technology is the state-of-the-art in IGA, its use in both design and analysis has not yet become mainstream. To provide a tool for more widespread adoption of T-splines based IGA, we created software plugins in both Rhinoceros 3D (Rhino) and Abaqus Unified FEA (Abaqus), two widely used software packages in design and analysis respectively. This integrated software solution has three primary steps: import/convert CAD or mesh data into a Rhino surface T-spline representation, convert surface T-spline representation into a volumetric T-spline representation, and IGA of T-spline volumetric elements in Abaqus through a custom User Element Subroutine (UELMAT). In order to encourage the adoption of T-splines in engineering design-through-analysis, our software solution eases designers into the use of T-spline technology by giving designers the flexibility of choosing from several common legacy CAD file formats to import into our software. This software supports the conversion of quadrilateral surface meshes, triangular surface meshes, trimmed and untrimmed NURBS surfaces and hexahedral meshes into T-spline surfaces/volumes. During the second step, the user refines the model and prepares it for analysis. The user can refine the entire mesh, adjust the model by manipulating “grip points”, and prescribe static loading and Dirichlet displacement boundary conditions. Lastly, a volumetric T-spline is constructed from the manifold T-spline surface geometry to enable analysis of the enclosed volume. In the final step, the finite element solution to the volumetric T-spline boundary value problem is determined in Abaqus via a custom T-spline UELMAT, and solution results are visualized in the Abaqus Viewer after post-processing. Keywords: Design-Through-Analysis, Rhino Plugin, Abaqus UELMAT, T-spline surface, solid T-spline construction, mesh conversion, trimmed NURBS conversion, isogeometric analysis, finite element analysis

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Title: Wave Velocity Dispersion and Spurious Reflections of Timoshenko's Flexural Waves

Author(s): Jose Laier, *São Carlos USP*.

Jose Elias Laier Engineering School of São Carlos (EESC), Department of Structural Engineering, University of São Paulo, São Carlos SP, Brazil, jelaier@sc.usp.br The finite element method is used to solve a wide range of engineering problems including wave propagation in elastic media. Because the finite element method is an approximation of a continuum medium, it is employed to solve wave motion results in appendant dispersion and spurious oscillations. Numerical wave velocity dispersion typically occurs in finite element solutions, where wave equations are first semi-discretized in space by the Galerkin methodology and then numerically integrated over time. Spurious wave reflections typically appear at the interfaces of elements with different lengths [1]. The proposed algorithm is formulated in terms of two Hermitian finite difference operators [2] with a fifth-order local truncation error [3]. Because the developed algorithm considers the repeated differentiation of the governing equations, additional nonlinear terms are required when solving nonlinear structural problems. Although the presence of these additional nonlinear terms increases the number of operations in the iterative operations and introduces some numerical noise, the reduction obtained in the matrix factorization and higher orders of the relative radii errors are interesting attributes of the proposed algorithm. The numerical results reveal that the proposed algorithm, which considers the dispersion of the lumped mass matrix results, are similar to results obtained by the Newmark Method, which considers a classical consistent mass matrix, for which the amount of operations is typically two times greater. Conversely, the spurious reflections can present significant magnitudes for even refined mesh. References [1] Bazant Z. P. Spurious reflection of elastic waves in nonuniform finite element grids, Comp Meth in Applied Mech Engng, 1978, 16, p.91-100 [2] Collatz L. The numerical treatment of differential equations, Springer-Verlag, 2nd Ed., 1966. [3] Laier JE. Mass lumping, dispersive properties and bifurcation of Timoshenko´s flexural waves. Adv Eng Software, 2007, 33, p. 605-610.

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July 27-30, 2015, San Diego, California, USA

Title: Isogeometric Implementation of the High-Order Microplane Model for Softening and Localization

Author(s): Gianluca Cusatis, *Northwestern U.* ; Erol Lale, *Northwestern U.*.

In this study, a recently developed higher order microplane (HOM) model for softening and localization, is implemented within a finite element framework based on isogeometric analysis. The HOM model was derived directly from a three dimensional discrete particle model and it was shown to be associated with a high order continuum characterized by independent rotation and displacement fields. Furthermore HOM model was demonstrated to possess two characteristic lengths: the first associated with the spacing of flaws in the material internal structure and related to the gradient character of the continuum; and the second associated with the size of these flaws and related to the micropolar character of the continuum. The displacement-based finite element implementation of this type of continua requires C1 continuity both within the elements and at the element boundaries. This motivated the implementation of the concept of isogeometric analysis which ensures a higher degree of smoothness and continuity. NURBS based isogeometric elements were implemented in a 3D setting and with both displacement and rotational degrees of freedom at each control point. The performed numerical analyses demonstrate the effectiveness of the proposed HOM model implementation to ensure optimal convergence in both elastic and softening regime. Particularly, the proposed approach prevents strain localization and spurious mesh sensitivity known to be pathological issues for typical local strain-softening constitutive equations.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Nitsche-XFEM Fictitious Domain Methods and Splitting Schemes for the Simulation of Thin-Walled Structures Immersed in an Incompressible Fluid

Author(s): Frédéric Alauzet, Benoit Fabrèges, Miguel A. Fernández, Mikel Landajuela, *INRIA*.

The use of fictitious domain/immersed boundary methods for the numerical simulation of fluid-structure interaction problems has recently seen a surge of interest. In this work we consider the extension of the Nitsche-XFEM method (see [1]) to fluid- structure interaction problems involving a thin-walled elastic structure (Lagrangian formalism) immersed in an incompressible fluid (Eulerian formalism). The fluid domain is discretized with an unstructured mesh not fitted to the solid mid-surface mesh. Weak and strong discontinuities across the interface are allowed for the velocity and pressure, respectively. The kinematic/kinetic fluid-solid coupling is enforced consistently using a variant of Nitsche's method involving cut elements. Robustness with respect to arbitrary interface/element intersections is guaranteed through a ghost penalty stabilization (see [2]). For the temporal discretization, several coupling schemes with different degrees of fluid-solid splitting (implicit, semi-implicit and explicit) are investigated. In particular, we address the extension of the explicit coupling paradigm introduced in [3] to the unfitted mesh framework. The stability and convergence properties of the methods proposed are rigorously analyzed in a representative linear setting. Several numerical examples, involving static and moving interfaces, illustrate the performance of the methods. [1] R. Becker, E. Burman and P. Hansbo. A Nitsche extended finite element method for incompressible elasticity with discontinuous modulus of elasticity. Comput. Methods Appl. Mech. Engrg, 198(41-44):3352–3360, 2009. [2] E. Burman and P. Hansbo, Fictitious domain methods using cut elements: III. A stabilized Nitsche method for Stokes problem. M2AN Math. Model. Numer. Anal., 48(3):859–874, 2014. [3] M. Fernández, J. Mullaert, M. Vidrascu, Explicit Robin-Neumann schemes for the coupling of incompressible fluids with thin-walled structures, Comput. Methods Appl. Mech. Engrg. 267 (2013) 566–593.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Numerical Simulation of Unsaturated Flow in Swelling Porous Media

Author(s): Nadia Laredj, Mustapha Maliki, Hanifi Missoum, Karim Bendani, *Abdelhamid Ibn Badis U.*.

Different models for the description of swelling pressure in clays have been proposed in recent years. Some models are based on geotechnical properties, these models are empirical, obtained from a statistical approach, others originated from concepts of thermodynamics and another class of models resulted from the diffusive double layer theory of Gouy and Chapman. The swelling characteristics are strongly influenced by the pore fluid chemistry and the mineralogical composition of clays. The composition of interlayer cations controls the interlayer water content. Hence, the saturated water content and the swelling pressure. This study presents the effect of osmotic potential due to chemical solute concentration changes via the use of the net stress, suction and chemical solute concentration elastic constitutive relationship. This model will represent the deformation behaviour exhibited by expansive clays. In particular, it was suggested that the determination of the stiffness of the soil with respect to chemical solute concentration could be achieved via a theoretical approach or by an empirical relationship. References: [1] Sridharan, A. et Prakash, K., (2000) “Classification procedures for expansive soils”. Proc. Instn. Civ. Engrs. Geotech. Engng, 2000, pp. 235-240. [2] Thomas, H. R. and He, Y., (1995) “A analysis of coupled heat, moisture and air transfer in unsaturated soil” Geotechnique, 45(4):677-689 [3] Bennethum, L., Murad, M.A., Cushman, J., (2000) “Macroscale thermodynamics and the chemical potential for swelling porous media” Transport Porous Med. 39, 187-225.

13th U.S. National Congress on Computational Mechanics
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Title: Arterial Stiffness and Left-Ventricular Function in a 3D Full-Body Scale Deformable Arterial Model

Author(s): Kevin D. Lau, C. Alberto Figueroa, *U. Michigan*; Nan Xiao, *King's College London*; Mahdi Esmaily-Moghadam, Alison L. Marsden, *UC San Diego*; Jay D. Humphrey, *Yale U.*.

Increases in arterial stiffness have been clinically shown to be an indicator of risk of fatal cardiovascular events such as stroke and heart attack [1]. The risk associated with arterial stiffening is typically assessed indirectly through the speed of blood pressure waves travelling throughout the arterial network (i.e. the pulse wave velocity). The faster the pulse wave velocity, the stiffer the arterial vessel and the greater the cardiovascular risk. However the specific correlation between abnormal increases in arterial stiffening and cardiovascular risk is still not fully understood. Computational models enable to quantitatively examine the relationship between variations in arterial stiffness throughout the arterial network and the corresponding pulse wave velocity. Using our in-house finite element software CRIMSON we are able to simulate blood flow in a given arterial geometry, under a range of different arterial stiffness that represent healthy, elderly (increased stiffness in all blood vessels) and diseased (localized stiffening) states of the arterial network. Analysis of the resulting hemodynamics provides further insight into the relationship between arterial stiffness, pulse wave velocity and the resultant workload on the heart. Based on medical images, we have built a model of the arterial system that includes the aorta and the main vessels of the head and neck, arms, and legs [2]. Consisting of a network of approximately 100 vessel, the resulting model was discretized into a finite element mesh consisting of approximately 52 million tetrahedral elements. Using this mesh, simulations of pulsatile blood flow have been performed on 4512 processors in parallel - resulting in the largest 3D, patient specific, full body scale, simulations of blood flow performed in the world to date. References: [1] Laurent et al., “Aortic Stiffness Is an Independent Predictor of All-Cause and Cardiovascular Mortality in Hypertensive Patients”, Hypertension. 2001; 37: 1236-1241 [2] Xiao et al. "Multi-Scale Computational Model of Three-Dimensional Hemodynamics within a Deformable Full-Body Arterial Network", Journal of Computational Physics. Vol 244, pp. 22-40

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Dimension-Independent Likelihood-Informed MCMC

Author(s): Kody Law, *KAUST*; Tiangang Cui, Youssef Marzouk, *MIT*.

Many Bayesian inference problems require exploring the posterior distribution of high-dimensional parameters that represent the discretization of an underlying function. This work introduces a family of Markov chain Monte Carlo (MCMC) samplers that can adapt to the particular structure of a posterior distribution over functions. Two distinct lines of research intersect in the methods developed here. First, we introduce a general class of operator-weighted proposal distributions that are well defined on function space, such that the performance of the resulting MCMC samplers is independent of the discretization of the function. Second, by exploiting local Hessian information and any associated low-dimensional structure in the change from prior to posterior distributions, we develop an inhomogeneous time-discretization scheme for the Langevin stochastic differential equation that yields operator-weighted proposals adapted to the non-Gaussian structure of the posterior. The resulting dimension-independent and likelihood-informed (DILI) MCMC samplers may be useful for a large class of high-dimensional problems where the target probability measure has a density with respect to a Gaussian reference measure. Two nonlinear inverse problems are used to demonstrate the efficiency of these DILI samplers: an elliptic PDE coefficient inverse problem and path reconstruction in a conditioned diffusion.

13th U.S. National Congress on Computational Mechanics
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Title: Topology Optimization of Composites Accounting for Non-Linear Interface Phenomena

Author(s): Matthew Lawry, Reza Behrou, Kurt Maute, *U. Colorado*.

When designing the layout of material systems composed of multiple phases by topology optimization, a perfect bond at the interfaces is typically assumed. While this assumption simplifies the structural model and circumvents the need for explicitly describing the interface geometry, it ignores interface phenomena that may dominate the structural response, such as contact, friction, and delamination. In this paper we study the influence of such interface phenomena on the optimum structural layout and composition of heterogeneous materials. To this end, we adopt a topology optimization method that describes the geometry by an explicit level set method (LSM) and predicts the structural response by the extended finite element method (XFEM). The combination of LSM and XFEM allows accurate resolution of interface geometry and related interface phenomena. The formulation of the optimization problem with focus on the structural and interface models is presented. We study two-phase optimization problems considering perfect bonding, adhesive bonding, and contact with and without friction. The optimization results demonstrate that interface phenomena may strongly influence the optimum design and that, in general, the interface conditions need to be accurately captured to obtain reliable optimization results.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Phase-Field Modeling of Biological Membranes

Author(s): Guillermo Lázaro, Ignacio Pagonabarraga, Aurora Hernández-Machado, *U. Barcelona* .

Biological membranes are characterized by a vanishing surface tension, so that their main elastic contribution is the bending. This feature determines the mechanic response of the membrane and hence it is important in many biological processes within the cell, such as cell deformation or vesicle formation. Phase-field models represent a powerful tool to study membrane phenomena [1], though the tensionless nature of these structures requires a deep understanding of the elastic properties of phase-field interfaces. We have developed a membrane phase-field model which allows us to study the elastic response of the membrane. We have shown its convergence to the Helfrich theory of membranes and application to different cell mechanics problems [2,3]. [1] G. R. Lázaro, I. Pagonabarraga and A. Hernández-Machado. (2015) Chem. Phys. Lip. 185: 46-60. [2] G. R. Lázaro, A. Hernández-Machado and I. Pagonabarraga. (2014) Soft Matter 10: 7195–7206. [3] F. Campelo and A. Hernández-Machado (2008). Phys. Rev. Lett. 100:158103.

13th U.S. National Congress on Computational Mechanics
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Title: Correcting the Surface Effect in Peridynamics: Applications to Elasticity, Fracture, and Material Interfaces

Author(s): Quang Le, *U. Nebraska-Lincoln*.

Peridynamics (PD) has been successfully used in modeling media with emerging and evolving discontinuities such as cracks [1, 2]. Based on an integro-differential formulation that does not use spatial derivatives of the displacement field, the theory remains mathematically consistent in the presence of cracks. In PD, a material point interacts with every point around it within a cut-off distance called the horizon. This domain of interaction is called the neighborhood. The derivation of micro-bond modulus and critical relative elongation in bond-based peridynamic formulation, and of the constitutive parameters in the state-based peridynamic model assume material points in the bulk. Therefore, the material point in these derivations has a “full neighborhood” of non-local interactions. At a boundary, however, a material point does not have this full neighborhood. If one uses the parameters derived for a point in the bulk, for the peridynamic bonds of points near the surface, in general, one observes that the effective stiffness of the material near the boundary is lower than that in the bulk. In addition, slight anisotropy near the surface is also present. This is called the “surface effect” in PD. In many cases, as the horizon size goes to zero, this effect can be neglected. However, taking the horizon to sufficiently small values for the effect to become negligible, leads to very high computational cost. In addition, for problems that have an inherent length-scale, the horizon size has to have a certain value and it cannot be taken to zero in the limit (see [3]). In order to resolve this issue and be able to compute accurate solutions in elasticity, for example, with any horizon size, methods for correcting the surface effect have been proposed recently. In this presentation, we discuss and compare several such approaches, in terms of elastic deformations of a plate and J-integral values for a plate with an edge-notch. We describe the advantages and disadvantages of each method and propose way for improving them. [1] S. A. Silling, Journal of the Mechanics and Physics of Solids, vol. 48, pp. 175-209, 2000. [2] S. A. Silling and E. Askari, Computers & Structures, vol. 83, pp. 1526-1535, 2005. [3] F. Bobaru and W. Hu, International Journal of Fracture, vol. 176, pp. 215-222, 2012.

13th U.S. National Congress on Computational Mechanics
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Title: Automatic Hexahedral Mesh Adaptation for Numerical Design

Author(s): Nicolas Le Goff, *CEA*.

Numerical modelling and design is a growing-up technology used in many manufacturing sectors (like automotive or aerospace for instance). Relying on computer-aided engineering techniques, which allows getting fast virtual prototyping, requires diminishing user's interaction and queries as much as possible. In this context, hexahedral mesh generation remains a bottleneck to overcome. More specifically, depending on the expected mesh quality, it can even be very time-consuming for engineers. In this work, we focus on the iterative design of CAD geometries, which are progressively refined by adding geometric details (chamfer, holes, etc.). Considering a meshed CAD model that we want to enrich, we adapt the initial mesh without having to regenerate it from scratch for each new 3D detail inserted into the model. Our method consists in classifying mesh entities to the new geometric part as follows: - First cells are classified to the new volume; this set of cells must meet some requirements such as being of the same genus as the inserted volume and being non-manifold. To better capture the part, the initial mesh can be locally refined using a 3-refinement scheme. We will then restrict ourselves to working on the surface of the selection; - Nodes are then classified to geometric vertices on a nearest basis; - Paths of edges linking end-nodes are classified to geometric curves using a shortest distance algorithm; - Patches of faces delimited by edges paths are classified to the surfaces depending on their delimiting curves. Once the geometric classification has been completed, a projection step is applied and layers of mesh elements are inserted since our method currently can associate for example two or more faces of a same cell to the same surface, thus producing badly-shaped elements. A smoothing phase is eventually applied. The main contributions of our work are: - Contrary to existing algorithms [Mar09, Zhang12], our method is not restricted to grids or octrees and can handle any unstructured meshes and elements (while focusing on hexahedral meshes we accept other kinds of elements); - We discretize both the inner and the outer volume. [Mar09] Marechal L., Advances in Octree-Based All-Hexahedral Mesh Generation: Handling Sharp Features. In proceedings of the 18th International Meshing Roundtable (2009). [Zhang12] Qian J. and Zhang Y., Automatic unstructured all-hexahedral mesh generation from B-Reps for non-manifold CAD assemblies. In Engineering with Computers (2012).

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: External Acoustic Scattering from Periodic Heterogeneous Media Using Analytical Techniques

Author(s): Jason Kulpe, Karim Sabra, Michael Leamy, *Georgia Tech*.

This talk will discuss advances made in analytically predicting acoustic scattering from finite-sized, periodic, heterogeneous media such as phononic crystals and acoustic metamaterials. First described is a Bloch Wave Expansion (BWE) technique [1] for determining the excited Bloch, decaying, and evanescent waves excited in the periodic media. This is coupled with reflected wave orders, treating the media as a periodic grating, which together satisfy continuity conditions at the interface of the incident media and the heterogeneous media. Next described is application of the Helmholtz-Kirchhoff Integral (HKI) theorem for predicting the external, scattered response. Finally, the performance of the combined BWE-HKI approach is assessed through comparison to solutions obtained using a Self-Consistent Scattering (SCS) approach. For frequencies within a bandgap, the BWE-HKI solution compares very well with the SCS solution, even for complex geometries requiring a facet-like discretization of the surface. The computation time, which is significant in both approaches, also points to an advantage for the BWE-HKI approach, especially considering it can be easily parallelized, unlike the scattering approach. References [1] Kulpe, J.A., Sabra, K.G., Leamy, M.J., 2014, “Bloch-Wave Expansion Technique for Predicting Wave Reflection and Transmission in Two-Dimensional Phononic Crystals,” Journal of the Acoustical Society of America, 135 (4): 1808-1819.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling Simultaneous Initiation and Propagation of Hydraulic Fractures Transverse to a Horizontal Wellbore

Author(s): Brice Lecampion, Jean Desroches, *Schlumberger*.

Multi-stage fracturing is the current preferred method of completing horizontal wells in unconventional hydrocarbon reservoirs. Its core component consists in simultaneously initiating and propagating an array of hydraulic fractures. We present a numerical model for the initiation and growth of an array of parallel radial hydraulic fractures. The solution accounts for fracture growth, coupling between elastic deformation and fluid flow in the fractures, elastic stress interactions between fractures and fluid flow in the wellbore. We also take into account the presence of a local pressure drop (function of the entering flow rate) at the connection between the well and the fracture, i.e. a choke-like effect due to current well completion practices, also referred to as entry friction. The partitioning of the fluid into the different fractures at any given time is part of the solution and is a critical indicator of simultaneous (balanced fluid partitioning) versus preferential growth. The numerical scheme is fully implicit. We use boundary elements and finite volume discretization for the solution of the elasto-hydrodynamics equation in the fractures. The location of the fractures front (and fracture velocity) is solved using a level set algorithm based on the general hydraulic fracture tip asymptotics. The fluid partitioning between fractures is solved for each trial location of the fracture fronts using a quasi-Newton scheme. We validate our numerical model against reference solutions and laboratory experiments for the initiation and growth of a single radial hydraulic fracture. We then investigate the impact of stress interaction on preferential growth of a subset of fractures in the array. Our results show that a sufficiently large local entry friction provides a strong feedback in the system and thus can counteract elastic stress interaction between fractures, therefore ensuring simultaneous growth. We propose a dimensionless number capturing the competition between stress interaction and local entry friction. This dimensionless number is a function of rock properties, fracture spacing and injection parameters. We verify that it captures the transition from the case of simultaneous growth (entry friction larger than interaction stress) to the case of preferential growth of some fractures (interaction stress larger than entry friction). We also discuss the implication of these results for multi-stage fracturing engineering practices.

13th U.S. National Congress on Computational Mechanics
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Title: Markov Chain Monte Carlo Samples for Bayesian Inverse of Structural Dynamic Systems

Author(s): Christophe Lecomte, *U. Southampton*.

The parameters of a structural dynamic system may be identified statistically, based on actual measurements of transfer functions. In a Bayesian context, the only things that need to be known in principle are the system likelihood, i.e. the probability of measurements for a given set of parameters, and the probability of these parameters prior to any measurements. Very complicated integrals would however be impossible to evaluate in practice in many situations and recourse to implicit methods is thus often privileged. Commonly used Markov Chain Monte Carlo (MCMC) methods are among such approaches that implicitly draw samples from the statistical probabilities of the parameters, posterior to measurements. The basic strategy behind MCMC is that one picks randomly a trial sample that is only accepted as a true sample with some probability. After some time – burn-in -, the chain of samples converges to samples that would equivalently have been drawn directly from the posterior. Rule of thumb conditions are that the trial samples are drawn neither too far nor too close from the last accepted sample, and that an acceptance rate of about thirty percent leads to such convergence. It is however shown here that these typical conditions do not work in the case of structural dynamic systems, in the sense that convergence may be practically impossible. The reasons for these difficulties are identified and it is explained that the absence of convergence may be entirely missed by an engineer using the common conditions blindly. The issues are fundamental and are hard to circumvent by traditional acceleration methods for systems whose measurements exhibit singularities. New sampling strategies are proposed and explored.

13th U.S. National Congress on Computational Mechanics
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Title: 3D Frame Fields: A Tool for Hexahedral Meshing

Author(s): Franck Ledoux, *CEA DAM*.

For many years, providing an algorithm to generate hexahedral meshes that fulfills minimal geometric criteria – boundary-alignment, minimum of singularity vertices – and that is not limited to a category of geometries has been an open issue, which is still unsolved. The major difficulty to overcome with hexahedral meshing is to consider the topological structure of the problem. Hexahedral meshes are structured in a global way: the topological structure of those is a simple arrangement of surfaces that traverse the whole mesh. This global structure prevents scientists and code developers to adapt traditional tetrahedral meshing or quadrilateral surface meshing algorithms, which are mainly based on local operations, to address the issue of hexahedral meshing. Generating hexahedral meshes requires solving a global geometrical and topological problem. For few years now, frame fields have been used by different research teams as a guideline to generate full-hexahedral or hex-dominant meshes. A 3D frame, which can be understood as being a triad, encapsulates the orientation of single hexahedral element. Gathered in a field, frames give continuous geometrical information that can drive the creation of hexahedral elements inside the volume to be meshed. Using this mathematical tool, many authors got encouraging results [Li12, Kow14, Ber14] but it is quite justified to ask if frame field is the right tool to pave the path towards automatic block-structured hexahedral meshing. This is the topic of this work, which starts with a comparison between 3D frame fields and the inherent topological structure of hexahedral meshes. Then we will see how frame fields are used in [Li12, Kow14, Ber14] to generate both full hexahedral meshes and hex-dominant meshes for geometric CAD models. Eventually, promises and limitations of these approaches will be given before addressing new directions for future research. [Li12] Y. Li, Y. Liu, W. Xu, W. Wang and B. Guo, All-hex meshing using singularity-restricted field, ACM Trans. Graph., vol. 31, pp. 1–11, 2012. [Kow14] N. Kowalski, F. Ledoux and P. Frey, Block-Structured Hexahedral Meshes for CAD Models using 3D Frame Fields, 23rd International Meshing Roundtable, Procedia Engineering, Elsevier, pp. 59-71, October, 2014. [Ber14] P.-E. Bernard, J.-F. Remacle, N. Kowalski and C. Geuzaine, Hex-dominant meshing approach based on frame field smoothness, 23rd International Meshing Roundtable, Procedia Engineering, Elsevier, vol. 82, pp. 175–186, October, 2014.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: On the Effects of Leaflet Microstructure and Constitutive Model on the Closing Behavior of the Mitral Valve

Author(s): Chung-Hao Lee, Michael Sacks, *UT Austin*.

Recent long-term studies showed an unsatisfactory recurrence rate of severe mitral regurgitation 3-5 years after surgical repair, suggesting that excessive tissue stresses and the resulting strain-induced tissue failure are potential etiological factors controlling the success of surgical repair for treating mitral valve (MV) diseases. We hypothesized that restoring normal MV tissue stresses in MV repair techniques would ultimately lead to improved repair durability through the restoration of MV normal homeostatic state. The accuracy of the MV computational model is critical for better understanding how MV tissue adaption maintains MV normal homeostasis in response to stress overload, pathologies and surgical intervention. Therefore, we developed, in this study, an anatomically accurate MV finite element model, which incorporated actual fiber microstructural architecture and a realistic structure-based constitutive model, for investigating the MV closing behaviors. Comparisons with extensive in-vitro data were made to validate the proposed model. Comparative and parametric studies were conducted to identify essential model fidelity and information for achieving desirable accuracy. More importantly, we, for the first time, investigated the interrelationship between the local fiber ensemble behavior and the organ-level MV closing behavior. Our findings demonstrated the appropriate parameter ranges and the underlying micro-mechanisms and microstructural adaption of the collagen fiber network for maintaining the proper coaptation and natural functioning of the MV under physiological loading. In addition, one of the main contributions in the present work was the acquisition of extensive in-vitro experimental data for thorough and rigorous validations of the accuracy of our models, and, in the meantime, the sample integrity was carefully maintained throughout the entire model development process, including micro-CT imaging, measurements of fiber microstructural architecture, and mechanical testing for the same ovine mitral valve specimen. We also demonstrated in the sensitivity study that a computational model with the highest model fidelity, in terms of leaflet microstructural information about local material axes and fiber splay dispersion, yielded the most accurate predictions in the displacement field as well as the strain field for the MV apparatus during systolic closure. These results underscored the necessary information to be included in the computational model for achieving the desirable accuracy and provide guidance in clinical practice by compromising between model simplification (efficiency) and simulation accuracy. The proposed computational model would serve as a logical first step toward our long-term modeling goal—facilitating simulation-guided design of optimal surgical repair strategies for treating diseased MVs with significantly enhanced durability.

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Title: Phase-Field Modeling for Hydraulic Fracturing in Porous Medium

Author(s): Sanghyun Lee, *UT Austin*; Andro Mikelic, Thomas Wick, Mary F. Wheeler, .

The computational modeling of the formation and growth of the fluid filled fractures in poroelastic media is difficult with complex fracture topologies. Here we study the fracture propagation by approximating lower-dimensional fracture surface using the phase field function. The major advantages of using phase-field modeling for crack propagation are i) it is a fixed-topology approach in which remeshing is avoided, ii) crack nucleation, propagation path are automatically determined based on energy minimization, and iii) joining and branching of multiple cracks also do not require any additional techniques. The study of phase field is form on the variational methods with energy minimization, which was studied by Buliga 1999, Francfort-Marigo 2000, Del Maso-Toader 2002, Bourdin 2008, and Miehe-Welschinger-Hofacker 2010. In addition, the phase field method coupling with pure elasticity and pressure was first studied by Fracfort-Marigo-Bourdin 2000-2008, Miehe-Hofacker-Welschinger 2010-2012, Borden Hughes et al 2012-2013, and Bourdin-Chukwudozie-Yoshioka 2012. However, the phase-field algorithms for fracture propagation in porous media have been developed in the last years by Mikelic, Wheeler and Wick 2013,2014. This work presents recent progress in phase-field-based fracture modeling in heterogeneous porous media. We develop robust numerical algorithms that can be used for three-dimensional applications. Specially, we present a Newton loop that combines a primal-dual active set method (required for treating the crack irreversibility) for pressurized fractures and couple this loop with a pressure-diffraction equation in order to solve for fluid flow in the porous media and the fracture. The resulting algorithm splits geomechanics and flow computations in terms of a fixed-stress approach. Several numerical examples considering pressurized fractures in heterogeneous media and fluid-filled fracture propagation in porous media substantiate our developments. This is a joint work with A.Mikelic, M.F.Wheeler, and T.Wick.

13th U.S. National Congress on Computational Mechanics
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Title: Multiscale Modelling of Multi-Physics: From Atom to Continuum

Author(s): James Lee, Jiaoyan Li, Zhen Zhang, *George Washington U.*.

Molecular dynamics (MD) and continuum mechanics (CM) are two distinct fields, very mature and successful in their own right. However, CM is invalid for material systems at nanoscale. On the other hand, even with a state-of-the-art supercomputer, MD is limited in the length/time scale that it can handle. Yet, our ultimate objective is to design and manufacture material systems in which organization is designed and controlled on length scales, with corresponding time scales, ranging from nanoscopic to microscopic, even to macroscopic. Therefore bridging the gap between MD and CM theoretically and numerically has become imperative and remains as a grand challenge. Consider a crystalline material system consisting of two regions (1) an atomic region: modeled by MD and a relatively small time step is used to update the solutions in time, and (2) an atom-based continuum region: modeled by coarse-grained molecular dynamics (CGMD) and a relatively large time step is employed to reduce the computational efforts. Since the crystalline material is distinguished from other states of matter by a periodic arrangement of the atoms, it can then be represented as a collection of repeated unit cells and a group of discrete and distinct atoms situated within each unit cell. The key point is how to calculate the interatomic force for both atomic region and atom-based continuum (ABC) region. In the ABC region, we assume the generic displacement field can be related to the corresponding nodal values through shape functions, similar to the situation in finite element analysis. We also prove that the interatomic forces at the nodes can be obtained through the interatomic forces at generic atoms. Correspondingly, we develop a multiple time scale algorithm. To control the temperature in specific atomic regions and/or ABC regions, an upgraded Nosé-Hoover thermostat is formulated. The electromagnetic effect is also included through the Lorentz force. One may calculate the electrical quantities, including polarization, voltage, and electrical field, based on atomic motions. It is noticed that temperature in continuum mechanics is an independent variable. Therefore one needs to save an energy equation; this is opposite to the situation in MD simulation. We will discuss the challenges if one wants to extend the multiscale simulation from atoms to genuine continuum.

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Title: Total Lagrangian Hydrocode for Linear Tetrahedral Elements in Compressible, Nearly Incompressible and Truly Incompressible Fast Solid Dynamics

Author(s): Chun Hean Lee, Antonio Javier Gil, Javier Bonet, Rogelio Ortigosa, *Swansea U.*.

Modern linear tetrahedral element technology in solid mechanics (e.g. ANSYS AUTODYN, LS-DYNA, ABAQUS, Altair HyperCrash), typically based on the use of the traditional second order displacement based formulation, possesses several distinct disadvantages, namely: (1) Reduced order of convergence for strains and stresses; (2) High frequency noise in the vicinity of shocks; (3) Stability issues associated with shear locking, volumetric locking and pressure checkerboard instabilities. To address the shortcomings mentioned above, a novel mixed momentum/strains formulation as a set of first order conservation laws, fulfilling numerical involutions, has been recently developed by the authors [1–3]. In this paper, an alternative set of entropy-based conservation laws, aligned with the classical framework of hydrodynamics, by using a mixed velocity/stresses formulation, is introduced. Crucially, the use of nearly incompressible polyconvex constitutive laws [3] ensures the physical existence of wave speeds. One of the key novelties is to introduce a Petrov-Galerkin stabilisation based fractional step method for polyconvex entropy formulations. This innovative idea, upon the work of Gil et al. [2], extends the range of applications towards the incompressibility limit without any volumetric constraints. A series of numerical examples are presented in order to assess the robustness of the proposed methodology. The overall scheme shows excellent behaviour in compressible, nearly incompressible and truly incompressible scenarios without any spurious hydrostatic oscillations and locking phenomena, yielding equal second order of convergence for velocities and stresses. References: [1] C. H. Lee, A. J. Gil and J. Bonet. Development of a stabilised Petrov-Galerkin formulation for conservation laws in Lagrangian fast solid dynamics. CMAME, 268, 40–64, 2014. [2] A. J. Gil, C. H. Lee, J. Bonet and M. Aguirre. A stabilised Petrov-Galerkin formulation for linear tetrahedral elements in compressible, nearly incompressible and truly incompressible fast dynamics. CMAME, 276, 659–690, 2014. [3] J. Bonet, A. J. Gil, C. H. Lee, M. Aguirre and R. Ortigosa. A first order hyperbolic framework for large strain computational solid dynamics. Part I: Total Lagrangian isothermal elasticity. CMAME, 283, 689–732, 2015.

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Title: Influences of Entrapped Air Voids on the Mechanical and Strengthening Characteristics of Sprayed Fiber Reinforced Polymer Composites: Micromechanics-Based Parametric Analysis

Author(s): B. J. Yang, H. K. Lee, *KAIST*.

In this paper, the structural behavior of reinforced concrete strengthened by SFRP composites is computationally investigated. A micromechanical constitutive damage model, which accounts for the void volume, is implemented into finite element code ABAQUS, and the overall strengthening performance of the system is predicted based on the proposed method. A comparison between numerical data obtained by FE code analysis and experimental results from four-point loading tests is discussed. ACKNOWLEDGEMENTS This research was supported by a grant (13SCIPA01) from Smart Civil Infrastructure Research Program funded by Ministry of Land, Infrastructure and Transport (MOLIT) of Korea government and Korea Agency for Infrastructure Technology Advancement (KAIA).

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Development of the Particle Difference Method for Solving Dynamic Crack Propagation Problems

Author(s): Kyeong-Hwan Kim, Sang-Ho Lee, *Yonsei U.*; Young-Choel Yoon, *Myongji College*.

This study presents a novel particle difference method (PDM) for solving dynamic crack propagation problems. The dynamic PDM yields a strong formulation by directly discretizing the governing partial differential equations. The numerical scheme is based on complete nodal computation using the Taylor polynomial expanded by the moving least squares procedure; it is free from any type of mesh or grid structure. Topology change due to crack growth, which is induced by a dynamic impact loading, is easily modeled by simplex nodal operation involving only partial rearrangement. Also, very efficient time integration algorithms are selectively adapted and newly developed for the dynamic PDM. The visibility criterion and dynamic energy release rate evaluation are combined with the dynamic PDM for crack propagation simulation. Numerical experiments thoroughly verified the accuracy and effectiveness of the developed method.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Stereographic Coordinates for Efficient High-Order Discontinuous Galerkin Finite Element Method

Author(s): Vincent Legat, *U. Catholique Louvain*.

An efficient approach is proposed to solve vectorial conservation laws on the sphere, using the stereographic projection and the Discontinuous Galerkin Method. This approach combines all the advantages of previous techniques described in the litterature. We describe a robust and accurate way to discretize partial differential equations on the sphere by means of the finite element method. The key idea is a dialog between the global coordinates of the vertices of an element and its local coordinates. This allows for the integration to take place on the stereographic plane instead of a curved space. The technique is validated on the sphere, using the shallow water equations for computing standard atmospheric benchmark. In particular, the Williamson test case is used to analyze the impact of the change of variables on the convergence rate for discretization error.

13th U.S. National Congress on Computational Mechanics
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Title: Reduced-Order Models of Structural-Acoustic Problems Using XFEM

Author(s): Antoine Legay, *CNAM*.

Noise reduction for passengers comfort in transport industry is now an important constraint to be taken into account during the design process. This leads to the study of several configurations of the structures inside a given acoustic cavity (optimization, uncertainty, ...). The classical finite element method needs an interface conforming mesh for each studied configuration which may become time consuming. The aim of this work is to be able to efficiently analyze different configurations of structures immersed in the acoustic domain and their influence on the noise level in the cavity. The thin flexible structures, with no thickness in the acoustic domain and discretized using shell elements, are immersed arbitrarily within the acoustic mesh allowing to always use the same acoustic mesh. This makes the parametric study easier since it does not involved a meshing process anymore. The first idea is to use XFEM in order to take into account the structure influences in the acoustic compressible fluid domain by enriching the pressure by a Heaviside function [1]. The finite element discretization of the whole fluid-structure coupled problem leads to a system in the frequency domain. In this system, the only matrices needed to be recomputed when the structures are placed arbitrarily in the fluid, are those corresponding to the enrichment and the one corresponding to the coupling between the fluid enrichment and the structures. The second idea is to build reduced basis. The structure basis is composed of its eigenmodes whereas a component mode synthesis with a fixed interface is used to build the fluid basis [2]. The interface degrees of freedom are thus the enriched nodes of the XFEM while the internal domain corresponds to the acoustic cavity with no structure. The method is implemented for shell structures embedded in a 3D fluid. The proposed approach is thus well suited for a parametric study of the structure positions in the fluid cavity with no re-meshing process, which is a significant saving in time. Further reduction strategies are currently investigated such as variable separation techniques. [1] A. Legay. An extended finite element method approach for structural-acoustic problems involving immersed structures at arbitrary positions. International Journal for Numerical Methods in Engineering, 93(4), 376-399, 2013. [2] A. Legay. The extended finite element method combined with a modal synthesis approach for vibro-acoustic problems. International Journal for Numerical Methods in Engineering, 101(5), 329-350, 2015.

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Title: A Moore-Penrose Continuation Method Based on a Schur Complement Approach for Non-Linear Finite Element Bifurcation Problems

Author(s): Sophie Leger, *U. Moncton*; Jean Deteix, André Fortin, *U. Laval*.

The finite element simulation of very large deformation of hyperelastic material is still a challenging problem. The problems are generally driven by a loading parameter and it is often observed that for some values of this parameter, the solution varies extremely rapidly due to geometric and/or material non linearities, often leading to the break down of the solution process. The typical solution strategy is often based on Newton like methods. The loading parameter is set to a given value, the Jacobian matrix stemming from the finite element discretization is constructed, the corresponding linear system is solved to correct the solution and this is repeated until convergence. The loading parameter is then somehow increased ("by hand") and the process is repeated until the total load has been imposed on the structure. In some situations, following the solution branch by increasing heuristically the loading parameter becomes extremely difficult and results in the divergence of the process. This is clearly the case in the neighbourhood of limit points or bifurcation points where the Jacobian matrix becomes singular. Numerical continuation methods have proved to be a very powerful tool when dealing with these kinds of problems. However, implementation of these methods often require modifications to the standard finite element method. As a finite element code is already very complex, we would like to implement the continuation method as efficiently as possible. In this paper, we present a new implementation technique based on a Schur complement approach for the Moore-Penrose continuation method. This method facilitates the detection of bifurcation points, which are associated with the critical loads leading to the sudden failure of the structure, and also enables branch following. Numerical examples will be presented and analyzed using the proposed approach.

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Title: An Efficient and Accurate Integration Scheme for Fictitious Domain Methods Based on Levelsets and Anisotropic Meshing

Author(s): Gregory Legrain, Nicolas Moës, *EC-Nantes*.

Fictitious domain methods allow to alleviate the meshing burden in numerical simulations, as they allow for the use of regular grids of elements. Among the methods used in solid mechanics, one can cite the Finite Cell Method [1], the eXtended Finite Element Method [2] and the Generalized Finite Element Method. The Finite Cell Method and the X-FEM, take advantage of very high order approximations (p-fem) so that very accurate solutions can be obtained even with coarse grids. For these higher order methods, a high geometrical accuracy is mandatory to achieve exponential convergence. Robust strategies based on sub-grid description of the interfaces were first considered, but unfortunately they lead to a large number of integration points. Alternatively, higher-order or exact mapping strategies have been considered with very good results. The main drawback of these strategies is the robustness of their extension to 3D complex (trimmed) geometries. In this contribution we propose an improvement of the computational efficiency of sub-grid descriptions. The strategy uses the levelset method for tracking the domain interface (like with the X-FEM). The tradeoff between geometrical accuracy and computational efficiency is obtained through the use of anisotropic mesh adaptation. An error estimator is used in order to drive the anisotropic mesh adaptation towards the interface. Furthermore, the elements tend to elongate along low curvature directions, which enables to decrease the number of elements for a given geometrical accuracy. Such a strategy allows to create an optimal geometrical mesh which is subsequently incorporated into the mesh defining the approximation. Finally, the efficiency of this method is demonstrated through various examples. Acknowledgements: The support of the ERC Advanced Grant XLS No 291102 is gratefully acknowledged [1] Parvizian J, Düster A, Rank E (2007) Finite Cell Method: h- and p- extension for embedded domain methods in solid mechanics. Comput Mech 41:122–133 [2] Moës N, Dolbow J, Belytschko T (1999). A finite element method for crack growth without remeshing. International Journal for Numerical Methods in Engineering 46 (1): 131–150

13th U.S. National Congress on Computational Mechanics
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Title: Quantifying the Influence of Conformational Uncertainty in Biomolecular Solvation

Author(s): Huan Lei, Xiu Yang, Bin Zheng, Nathan Baker, *Pacific Northwest Nat'l. Lab.*; Guang Lin, *Purdue U.*.

Biomolecules exhibit conformation fluctuations near equilibrium states, inducing uncertainty in various biological properties. We have developed a general method to quantify the uncertainty of target properties induced by conformation fluctuations based on generalized polynomial chaos expansion. To alleviate the high dimensionality of the conformation space, we propose a method to increase the sparsity of the gPC expansion by defining a set of collective variables within active subspace, which further increase the accuracy of the surrogate model based on compressive sensing method. The method is demonstrated on solvation properties and shown to yield a more accurate response surface than standard sparse grid collocation methods. Our framework is generalizable and can be used to investigate uncertainty in numerous biomolecular properties.

13th U.S. National Congress on Computational Mechanics
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Title: Lie Group Variational Integrators for Spacecraft with Variable Speed Control Moment Gyros

Author(s): Taeyoung Lee, *George Washington U.*; Frederick Leve, *Air Force Rsch. Lab*; Melvin Leok, *UC San Diego*; N. Harris McClamroch, *U. Michigan*.

A control moment gyroscope (CMG) is an attitude control actuator for a rigid body. It consists of a spinning rotor and motorized gimbals. By rotating the spin axis of the rotor, the angular momentum of the rotors is used to control the attitude of the rigid body. Compared with reaction wheels that apply torque by changing the rotor spin rate, a CMG is substantially more efficient and responsive. As such, it has been applied for various large spacecraft systems, including the international space station. However, it is challenging to analyze and simulate the dynamics of CMG systems accurately. For example, spacecraft actuation faults typically occur slowly over many years. This requires that the dynamics of a spacecraft with a CMG should be propagated over a long-time period accurately and efficiently. The existing dynamic models for a CMG rely on several simplifying assumptions, such as axially-symmetric mass distribution of the rotor; this assumption is in conflict with the need to model various fault scenarios. Furthermore, conventional numerical integration schemes, such as the popular variable stepsize Runge–Kutta methods, have undesirable long-term numerical properties. The first objective of this paper is to provide a comprehensive analytic model for a spacecraft with variable speed CMG. The configuration space is identified as a Lie group, and an intrinsic form of Euler-Lagrange equations are derived according to Lagrangian mechanics that are globally valid, without relying on simplifying assumptions. The second objective is focused on constructing a geometric numerical integrator, referred to as Lie group variational integrator, that provides long-term structural stability and reliability in simulating the CMG dynamics accurately. It has the unique desirable properties of preserving both the nonlinear configuration manifold structure and the Hamiltonian characteristics. It completely avoids singularities that appear in any local parameterization. These features are particularly useful to study complicated maneuvers of spacecraft with a CMG over a long time period, while exactly capturing the nontrivial dynamic coupling effects between the translational motion and the rotational motion of the spacecraft with various CMG designs. These features are illustrated by numerical examples.

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Title: High-Dimensional Uncertainty Quantification and Learning Backward in Time

Author(s): Pierre Lermusiaux, *MIT*.

Bayesian nonlinear state estimation and model learning of high-dimensional nonlinear fluid and ocean dynamical systems, both forward and backward in time, is developed. The Bayesian nonlinear smoothing combines reduced-order Dynamically-Orthogonal (DO) equations with Gaussian Mixture Models (GMMs), extending linearized backward pass updates to a Bayesian nonlinear setting. The approach is then utilized to learn properties of the dynamical modeling systems, propagating the information contained in present measurements backward in time. Examples are provided for fluid and ocean flows. This is joint work with our MSEAS group at MIT.

13th U.S. National Congress on Computational Mechanics
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Title: Simulation of Brittle Fracture Propagation with Universal Meshes

Author(s): Adrian Lew, *Stanford U.*.

We discuss recent advancements we have made in the simulation of brittle crack propagation with Universal Meshes. These include the computation of elastic solutions and associated stess intensity factors on cracked domains to any order of accuracy, and their use to compute convergent crack paths. Fundamental to these developments is the notion of a universal mesh, which enables us to slightly modify the same underlying mesh to always conform to the evolving crack geometry. We will show examples involving: (a) crack propagation in a rapidly-cooled glass slab, and (b) a curvilinear hydraulic fracture.

13th U.S. National Congress on Computational Mechanics
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Title: A Multi-Scale Micromorphic Molecular Dynamics (MMMD)

Author(s): Shaofan Li, *UC Berkeley*.

In this work, a con-current multiscale micromorphic molecular dynamics (MMMD) is proposed, formulated, and developed, which generalizes the classical Andersen-Parrinello-Rahman molecular dynamics to inhomogeneous systems with arbitrary finite domains. More importantly, it can take into account the macroscale continuum boundary condition as the input of molecular dynamics. The multiscale molecular dynamics is a con-current coupling of the fine scale molecular dynamics with a coarse scale finite element based nonlinear mesoscale continuum dynamics. By choosing proper closure conditions, we have shown that the Andersen-Parrinello-Rahman molecular dynamics is a special case of the proposed multiscale molecular dynamics. In other words, we have shown that the Andersen-Parrinello-Rahman molecular dynamics can be rigorously formulated and justified from first principle. Moreover, we also show that one may be able to derive the basic equations of nonlinear mesoscale continuum mechanics from first principle. Furthermore, the con-current multiscale continuum-molecular dynamics provides a solid foundation for general non-equilibrium molecular dynamics. To implement this con-current multiscale formalism, we have developed a three-dimensional multiscale continuum-molecular dynamics computer code, which couples the Parrinello-Rahman (PR) molecular dynamics with non-linear finite element based continuum dynamics. In this presentation, we shall present several numerical examples of the proposed MMMD to demonstrate the validity as well as the applications of the proposed multiscale method.

13th U.S. National Congress on Computational Mechanics
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Title: Bridging Different Length and Time Scales in Dusty Disk-Planet Interaction Simulations

Author(s): Shengtai Li, *Los Alamos Nat'l. Lab.*.

We present a multi-scale and multi-physics simulation tool for dusty proto-planetary disks. The disk motions are simulated by solving hydrodynamics equations (Navier-Stokes equations) for the coupled dust and gas fluids, where the dust particles are treated as pressureless fluid. The embedded planets are described by Newton's Law as N-body problems. Several length and time scales need to be solved simultaneously in the tightly coupled planet, dust and gas motions. We present several numerical techniques to bridge different scales and achieve comparable accuracy. These techniques include efficient semi-Lagrangian approach to alleviate the CFL limitation on time steps in disk motions, sub-cycling between fast and slow dynamics motions between disk and planets, partial equilibrium state to obtain reduced order model (ROM) and locally parallel-in-time method for the coupled stiff dust and gas dynamics, and Lagrangian adaptive mesh refinement to resolve the flow near the planet. Numerical examples are provided to demonstrate the effectiveness of our numerical methods.

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Title: An Atomistic Field-Theory for Ferroelectric Nanostructure Modeling

Author(s): Xiaowei Zeng, Meng Li, *UTSA*.

Intense experimental and computational effort has been made recently in understanding ferroelectric nanostructures because of their promise in increasing ferroelectric nonvolatile-memory density. The ferroelectric nanostructures are also critical in light of miniaturizing piezoelectric transducers and actuators, ultrasonic devices, and medical imaging detectors. The purpose of this research is to investigate the ferroelectric properties of nanoparticles, in particular, to explore the ferroelectric properties in nanostructures and how these nanostructures respond to applied electric field. An atomistic field theory will be presented to study the nanostructures. The field theory connects mechanical displacement directly to electric polarization from atomistic perspective. The polarization of a unit cell in a nanoscale ferroelectric perovskite can be calculated from atomic displacement. From the simulation, the microscopic paths by which homogeneous polarization switching process takes place in a ferroelectric perovskite are characterized. Molecular dynamics simulations are also performed to investigate the electromechanical response of a ferroelectric perovskite under finite temperature and electric field.

13th U.S. National Congress on Computational Mechanics
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Title: Reformulation of Nosé-Hoover Thermostat for Heat Conduction Simulation at Nanoscale

Author(s): Jiaoyan Li, James Lee, *George Washington U.*.

When Molecular Dynamics was originally conceived, the trajectories of atoms are determined by numerically solving the Newton's equations for a system under equilibrium condition. The revolutionary Nosé-Hoover dynamics modified Newtonian dynamics so as to reproduce canonical and isobaric-isothermal ensemble equilibrium systems. However, there is an increasing interest in conducting MD simulation for a nonequilibrium system whose temperature varies spatially and temporally with the imposition of a temperature gradient. Clearly, this is a heat conduction problem and requires Nonequilibrium Molecular Dynamics with suitable algorithmic thermostat for local temperature regulation. Inspired by Nosé-Hoover thermostat, this work reformulates the feedback force caused by the temperature control, aiming at (i) controlling the temperature locally at several distinct regions, and (ii) eliminating the rigid-body translation and rotation which are irrationally introduced into the system due to the temperature force. This reformulation will generate accurate and rigorous trajectories of atoms and thus the heat conduction can be performed successfully at nanoscale. Correspondingly, the definition of temperature is modified; the expression of Hamiltonian is upgraded. To demonstrate the capability and feasibility of this new algorithm, we studied heat conduction phenomena in a beam-like and a ring-like finite size specimen by using our in-house developed computer code. The results from the reformulated Nosé-Hoover thermostat show the temperature distributions across the specimens for long time duration until the steady state arrives. Yet, the results from the original Nosé-Hoover thermostat cannot yield the steady state solution. Also, it reaches the conclusion that the heat conduction at nanoscale exhibits the same feature of Fourier's law at macroscopic scale if the temperature is averaged over spatial region and a sufficiently large time interval. The thermal conductivity can thereafter be calculated based on the linear relation between the heat flux and the temperature gradient. It is found that the obtained numerical value of thermal conductivity matches the experimental result very well.

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Title: Numerical Comparison and Optimization of Functionally-Graded Structures Under Multiple Impact Loads

Author(s): Guangyong Sun, Zheshuo Zhang, Guangyao Li, *Hunan U.*; Jianguang Fang, Qing Li, *U. Sydney*.

Marketing pressure and ecological awareness force automobile manufacturers to achieve a highest possible product quality without increasing the weight of vehicles. This paper aims at promoting crashworthiness of vehicle's energy-absorbing components while maintaining its weight, by comparing the crashworthiness performance of functionally-graded thin-wall tubes under multiple load cases, which include hollow uniform thickness, hollow functionally graded thickness, foam-filled uniform thickness and foam-filled functionally graded thickness (F-FGT) configurations. Finite element (FE) analysis is used to simulate the crashing behavior and energy-absorbing capability. At first, the FE models are validated to ensure their accuracy by comparing with the experimental results and the close-form formula summarized from experiment. Then, a set of functionally-graded thin-wall tubes under multiple load cases are conducted and the results reveal that the F-FGT tube has the best crashing performance under multiple load cases considered. Further investigation into various patterns of wall thickness of the F-FGT tube indicates that the thickness gradient and thickness range significantly influence its crashworthiness under multiple impacting angles. And then, the Non-dominated Sorting Genetic Algorithm (NSGA-II) is used to seek for an optimal thickness variation for maximizing specific energy absorption and minimizing initial peak force under multiple loading angles. The optimal design of the F-FGT tube demonstrates better crashworthiness characteristics than those of other three optimal tube configurations, indicating that the F-FGT tube can be a potential energy absorber when oblique impact loading is inevitable.

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Title: Dynamic Crashing Behaviour of New Extrudable Multi-Cell Tubes with Functionally Graded Thickness

Author(s): JIANGUANG FANG, Qing Li, *U. Sydney*; Yunkai Gao, *Tongji U.*; Guangyong Sun, *Hunan U.*.

Multi-cell structures have been extensively studied as potential energy absorbers for their outstanding performance. Unlike existing multi-cell tubes with uniform thickness (UT), this paper introduces functionally graded thickness (FGT) to multi-cell tubes under dynamic impact, which can be fabricated by an extrusion process. Numerical model is established using nonlinear finite element analysis code LS-DYNA by validating against the experiment. Through the numerical study, thickness gradient parameters in different regions are found to have considerable effect on the crashworthiness of FGT multi-cell tubes. Moreover, FGT multi-cell tubes enable to absorb more energy whilst yielding similar level of peak impact force, compared with UT multi-cell tubes. Finally, the multiobjective optimizations of UT and FGT multi-cell tubes are conducted to seek the optimal gradient parameters to improve the specific energy absorption (SEA) and reduce the maximum impact force simultaneously, in which the multiobjective particle optimization (MOPSO) algorithm and response surface (RS) surrogate modeling technique are adopted. The optimization results demonstrate that the FGT multi-cell tubes produce more competent Pareto solutions than the conventional UT counterparts; and similar gradients in different regions of FGT multi-cell tubes are recommended attributable to their better interactions.

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Title: Non-Linear Dynamic Analysis for Building Structures Based on the Force Analogy Method

Author(s): Gang Li, Yongqiang Jin, Jialong Li, Feng Zhang, *Dalian U. Tech.*.

The force analogy method (FAM) is an analytical tool for solving structural analysis problems with material nonlinearity. It uses the concept of “inelastic displacement”, or more commonly known as the “residual displacement” in the formulation, where the nonlinear stiffness force due to material nonlinearity is represented by a change in displacement instead of a change in stiffness. In this study, a reinforced concrete shear-wall framed building structure was analyzed under earthquakes with the FAM. The results showed that the FAM is capable of simulating the nonlinear response of RC structures, including the material and geometric nonlinearity and the advantages of the proposed method are high efficiency and stability.

13th U.S. National Congress on Computational Mechanics
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Title: A Multi-Scale Generalized FEM for the Simulation of Spot Welds in Large Structures

Author(s): Haoyang Li, C. Armando Duarte, *U. Illinois, Urbana-Champaign*.

Spot welds are commonly used to join thin gauge metallic structural components of automotive and aerospace vehicles. The failure of spot welds in these components may lead to the catastrophic loss of the structure. Hence, modeling spot welds and resolving the local stress fields with high fidelity is important. There are currently several approaches for modeling spot welds. The representation of welds in the FEM involves the introduction of a few elements to represent the welded area. This approach provides some basic information about the local stress distribution. If a more accurate representation is desired, it requires a detailed meshing of each spot weld, leading to very fine computational models. This translates into rather extensive time spent on building the FEM model and on its solution, which is further compounded if parametric studies and modifications are required. Another common approach is to use Rigid Elements or Multi-Point Constraints which are introduced as point-to-point representations of the actual connectors. This simplistic solution serves the purpose of connecting thin structures, but it does not provide a good representation of the stiffness of the connection and practically no useful information about the stresses around the spot weld. The disparate scales involved in a large structure with hundreds of spot welds prevent one from having all the spot welds represented within a single model. It is not only because of the extensive computational cost, but also by the difficulty of generating such a mesh. We propose a Generalized Finite Element Method with global-local enrichment (GFEMgl) to resolve the spot weld problem. This GFEMgl is a multiscale framework which uses the solution of a local problem defined for each spot weld as enrichment functions for the structural-scale model. This methodology offers great flexibility. It allows the discretization of each spot weld independent of each other using fine meshes, while keeping the global mesh fairly coarse. In addition, the GFEMgl allows the adoption of different element types in global and local models. Thin gauge panels are more conveniently discretized by hex elements while tetrahedrons are more suitable for modeling the complex geometry at the spot weld scale. Numerical experiments show that the accuracy of the proposed GFEMgl is comparable with that provided by a direct numerical simulation with the fine-scale features discretized in the global mesh. This user-friendly GFEMgl also provides very good computational efficiency by exploring the natural parallelization of local problem computations.

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Title: Two Approaches for Solving Stochastic Variational Inequality Problems in the Framework of Polynomial Chaos Expansions

Author(s): Jianyu LI, *Tianjin U. Sci. & Tech.*; Roger Ghanem, *U. Southern California*.

Two approaches will be discussed to solve the stochastic variational inequality (SVI) problems in the framework of polynomial chaos expansions (PCE). One approach is called alternating projection approach, which is designed to solve the point-wise type of SVI, another approach is called semi-infinite programming approach, which is employed to solve the integral form of SVI. In the first approach, after representing SVI in the framework of PCE and using the equivalent projection equation formulation of VI, the solution of SVI is cast to a projection onto the interaction of a constraint set and a linear subspace spanned by PC, this perspective results in an alternating projection algorithm being designed to solve SVI. In the second approach, after representing SVI in the framework of PCE and using the equivalent optimization formulation of VI, the solution of SVI is the same as a solution of semi-infinite programming problem, based on this view of point, the algorithms already developed in the field of mathematical programming for semi-infinite programming problem is employed to solve SVI. Two specific applications in engineering, i.e. contact mechanics analysis and elastoplastic analysis, will be described to illustrate the main idea of those two approaches.

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Title: Variational Multi-Scale Analysis of Stochastic Partial Differential Equations

Author(s): Jason Li, Assad Oberai, Onkar Sahni, *RPI*; Jayanth Jagalur-Mohan, *MIT*.

We present the variational multiscale (VMS) method for stochastic PDEs to compute an accurate solution in a coarse physical and stochastic space while accounting for the missing scales through a model term. This fine-scale model term is defined by an approximation of the fine-scale stochastic Green's function. We consider an algebraic approximation for this model term based on a stabilization parameter (i.e., the residual-based variational multiscale method). The resulting stabilization parameter turns out to be a rational function of the random variables. When generalized polynomial-chaos (gPC) expansions are used to represent the solution in the stochastic space, the stabilization parameter is also approximated in the form of a gPC expansion. This allows us to exploit the well-documented properties of the gPC basis in constructing the underlying variational formulation. The gPC expansion for the stabilization parameter is obtained after constructing efficient projections for multiple operations that include division and fractional powers. We demonstrate the effectiveness of the VMS approach and the gPC expansion of the stabilization parameter for multiple problem cases. These include the advection-diffusion equation in multiple dimensions in the physical and stochastic spaces, where both the advective and diffusive regimes are attained. We also consider a more general problem case, where we study the transport of a species in a network of channels. This network is composed of many branches, where the incoming velocity for each branch is stochastic resulting in a high-dimensional stochastic problem.

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Title: On Error Estimation of the Stochastic Perturbation Method for Random Media

Author(s): Xiangyu Wang, Chenfeng Li, *Swansea U.*; Song Cen, *Tsinghua U.*.

Over the past few decades, Stochastic Finite Element Methods (SFEM) have been developed for numerical analysis of uncertainty propagation in various engineering applications, in which the random factors can arise from the geometry, the material properties or the boundary conditions. Unlike the conventional finite element method which has a well established theoretical framework, the SFEM has many different formulations, and these include the Monte Carlo method, the perturbation method, the Neumann expansion method, the polynomial chaos expansion method, and the joint diagonalization method, among others. Despite these developments, little work has been done to address the error estimation of SFEMs. This work focuses on the error estimation of the stochastic perturbation method. The basic idea and the development of the stochastic perturbation method is briefly recapped below. We also summarize the Monte Carlo method, which is taken as the reference for the error estimation. Despite the wide use in various applications, the perturbation method does not have a rigorous error estimation. Instead, the solution errors are usually examined by comparing with the Monte Carlo method. Purely based on experience, some papers suggested an applicable variation range of ten percent. Without rigorous proof, it is generally agreed that the perturbation method is has very good efficiency and accuracy for small random fluctuations, but the solution accuracy will decrease dramatically as the variation gets larger. This work addresses the a priori error estimation for the stochastic partial differential equations commonly encountered in stochastic finite element methods. For the first time, a priori error estimation is established for the stochastic perturbation method. The mathematically rigorous result is derived for the linear stochastic equations commonly encountered in stochastic finite element methods. Specifically, the error of the solution vector is directly linked to the variation range of the source stochastic fields, which can be computed a priori. Although the result is presented for examples with random elastic modulus, the concept is applicable to other more general cases, where the material parameter is linear with respect to the element stiffness matrix and the deterministic part (i.e. the expectation part) of the stiffness matrix is positive definite. The error of elastic-modulus homogenization for heterogeneous materials, which is identical to the zero order perturbation, is also discussed in this work.

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Title: Molecular Simulation Guided Constitutive Modeling on Finite Viscoelasticity of Elastomers

Author(s): Ying Li, Wing Kam Liu, *Northwestern U.*; Shan Tang, *Chongqing U.*; Martin Kroger, *ETH Zurich*.

A predictive multiscale computational framework has been developed to study the ■nite viscoelastic properties of elastomers. Using the Inverse Boltzmann Method [1, 2], both the static structures and dynamic behavior of all-atomistic models of elastomers can be reproduced by a simple coarse-grained model, which bridges the scale from nano to meso. On this coarse-grained level, the entangled network of elastomers is described via a primitive path analysis (Z1 code) [2]. This description allows extraction of the tube diameter and primitive chain length, quantities required to bridge the scale from meso to micro. Furthermore, by making the a■ne-deformation assumption, a continuum constitutive law for elastomers has been developed from the tube model of primitive paths, which bridges the scale from micro to macro. In this way, the di■erent scales are crossed by using di■erent bridging laws, which enable us to directly predict the viscoelastic properties of elastomers using a bottom-up approach. Our predicted dynamic moduli, zero-rate shear viscosities, and relaxation moduli of natural rubbers are found to be in excellent agreement with experimental results [2]. The developed multiscale computational framework can also be naturally extended to the ■nite deformation regime [3]. Both the tube diameter app and primitive chain length Lpp are found to increase with deformation, which enhances the viscous energy dissipation of elastomers under extremely large deformations [2]. To the authors knowledge, this is the ■rst work in which a multiscale computational framework has been proposed to predict the ■nite viscoelastic properties of elastomers from the molecular level. Not only can the method put forth in this research be used to predict the viscoelastic properties of elastomers in a bottom-up fashion, it can also be applied to design the elastomers with targeted functions, within a top-down approach. [1] Li, Y., Kroger, M. and Liu, W.K., 2011. Primitive chain network study on uncrosslinked and crosslinked cis-polyisoprene polymers, Polymer, 52:5867-5878. [2] Li, Y. , Tang, S. , Abberton, B.C. , Kroger, M. , Burkhart, C. , Jiang, B. , Papakonstan¬topoulos, G.J. , Poldne■, M. and Liu, W.K., 2012. A predictive multiscale computational framework for viscoelastic properties of linear polymers, Polymer, 53:5935-5952. [3] Li, Y. , Abberton, B.C. , Kr¨oger, M. and Liu, W.K., 2013. Challenges in Multiscale Modeling of Polymer Dynamics, Polymers 5 (2): 751-832.

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Title: EigenErosion: A Variational Fracture Algorithm in Mesh-Free Methods

Author(s): Bo Li, *Case Western Reserve U.*; Anna Pandolfi, *Politecnico di Milano*; Michael Ortiz, *Caltech*.

In the present work, we developed a variational material point failure algorithm (EigenErosion) as an extension of the EigenFracture scheme [1] to predict fracture and fragmentation in brittle and ductile materials [2]. In the EigenErosion approach, the eigendeformation, to be either zero or equal to the displacement gradient, is introduced as an internal variable to describe the local state of a material point or integration point. In addition, an energy release rate is defined at each material point by averaging the effective energy-release in an epsilon-neighborhood and compared to the material critical energy release rate for the failure of the material point. As an energy-based variational fracture algorithm, the eigenfracture scheme is known to properly converge to Griffith fracture in the limit of vanishingly small mesh sizes. In particular, the local-neighborhood averaging of the energy has the effect of eliminating spurious mesh-dependencies. Based on the optimal scaling analysis, the crack propagation modeled in the EigenErosion scheme is characterized by a simple parameter, the critical energy release rate, which greatly facilitates material characterization. To this end, the EigenErosion approach has been implemented within the Optimal Transportation Meshfree (OTM) framework [3] and extensively validated in our three dimensional simulations of three-point-bending tests on high strength concrete, Taylor impact experiments of polyurea, explosive loading and ballistic/hypervelocity impact tests on metallic targets by comparing against experimental measurements. [1] B. Schmidt, F. Fraternali, and M. Ortiz. Eigen-fracture: an eigendeformation approach to variational fracture. SIAM Journal on Multiscale Modeling and Simulation, 7: 1237–1266, 2009. [2] B. Li, A. Pandolfi, M. Ortiz, Material-Point Erosion Simulation of Dynamic Fragmentation of Metals, Mechanics of Materials, 80: 288-297, 2015. [3] B. Li, F. Habbal and M. Oritz, Optimal Transportation Meshfree approximation schemes for fluid and plastic flows, International Journal for Numerical Methods in Engineering, 83: 1541-1579, 2010.

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Title: A Mixed Finite Element - Crushable Discrete Element Nested Method for Granular Materials

Author(s): Xikui Li, Zenghui Wang, Yuanbo Liang, Qinglin Duan, *Dalian U. Tech.* .

A Mixed finite element (FE) - crushable discrete element (DE) nested method in the frame of the second-order computational homogenization for granular materials is proposed. Granular material is modeled as gradient Cosserat continuum at the macro-scale and a mixed FE for gradient Cosserat continuum is constructed based on the Hu-Washizu variational principle [1,2]. Patch tests are designed and performed to validate the mixed FE formulations. The complex macro-mechanical behavior of granular material are encoded at the grain scale. Hence granular material is modeled as discrete particle assembly for each meso-structural representative volume element (RVE) assigned to integration points of the mixed FE. A crushable discrete element model (CDEM) is proposed to investigate meso-mechanisms of macroscopic failure of granular material; i.e., not only dissipative inter-particle displacements, the loss and generation of particle contacts, but also particle breakage, at the meso-scale. The crushing criteria and fracture modes of individual particles for the proposed CDEM are investigated. The downscaling and upscaling rules to perform the two way coupling between the macro-scale using the mixed FE simulation and the meso-scale using the CDEM simulation are specified. The downscaling determines the micro-scale boundary value problem of the RVE with the given macroscopic strain measures via enforcement of the RVE boundary conditions in light of the generalized Hill's lemma [2]. The upscaling transited back the stress measures of the higher scale and the meso-mechanically informed macroscopic constitutive model from volume average of the sub-scale solution to the gradient Cosserat continuum. The performance of the mixed FE - crushable DE nest method in the simulation of strain softening and localization phenomena are demonstrated, without need to specify macroscopic phenomenological constitutive relationship and material failure model. References: 1. Belytschko T, Liu WK, Moran B. Nonlinear Finite Elements for Continua and Structures 2000, Wiley. 2. Li XK , Liang YB, Duan QL, Schrefler BA, Du YY. A mixed finite element procedure of gradient Cosserat continuum for second-order computational homogenisation of granular materials, Computational Mechanics 2014;54:1331–1356. 3. Li XK, Zhang X, Zhang JB. A generalized Hill's lemma and micro-mechanically based macroscopic constitutive model for heterogeneous granular materials. Comput Methods Appl Mech Engrg 2010; 199:3137-3152.

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Title: Thermal Transport and Fracture Behavior of Sintered Fuel Pellets: Interaction Between Experiment and MARMOT Fuel Modeling

Author(s): Jie Lian, *RPI*.

The advanced ceramic fuel development program is exploring revolutionary ceramic fuels with the potential of “game-changing” impact on reactor operation & response to beyond design scenario. Key properties of advanced fuels include high thermal conductivity, oxidation resistance, high temperature mechanical properties, and thus improved accident tolerance. Composite ceramic fuels possess distinct advantages to fulfill these key requirements. On the other hand, the US Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing science-based next generation fuel performance modeling capability as part its Fuel Product Line in order to facilitate the predictive capability of nuclear fuel performance and assist the design and analysis of reactor systems. Critical experimental data are needed to validate MARMOT models, particularly on effective thermal conductivity and fracture behavior and how microstructure features affect thermo-mechanical properties of fuels. The fabrication of sintered fuel pellets with well-controlled microstructure is prerequisite to establish the correlation of the microstructure feature and fuel behavior. In this talk, recent advancements of using field-assisted sintering technologies, specifically spark plasma sintering (SPS), in fabricating advanced fuels and engineering fuel matrix, providing as realistic initial microstructure for fuel microstructure modeling will be focused. The fuel behaviors are characterized with the focus on the thermal-mechanical properties and accident tolerance. The sintering fuels by SPS include monolithic UO2 with well controlled microstructure, grain size and porosity across multiple length scales from nano-metered to micron-sizes, and the impact of the microstructure on the fuel properties is discussed within the context of the MARMOT predictions.

13th U.S. National Congress on Computational Mechanics
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Title: Spatial Fractional Advection-Dispersion Equation Based on A Meshfree Method

Author(s): Yanping Lian, Gregory J. Wagner, Wing Kam Liu, *Northwestern U.*.

Anomalous diffusion phenomena can be observed in complex and important science and engineering problems, such as turbulent flow, contaminant transport in ground water, solute transport in porous media, and so on. These problems are often successfully described by partial differential equations (PDEs) with fractional derivatives requiring fewer parameters than corresponding integer-order derivative models. This is because the integral-differential definition of the fractional derivative can account for time effects, path-dependence, and global correlation in a natural way. Therefore, more and more attention has been paid to develop numerical methods for fractional PDEs. Due to the non-local property of the fractional derivative operator, for large-scale or long time history problems it is a challenge to build accurate and efficient numerical formulations based on current numerical methods, such as finite difference methods, finite element methods, or meshless methods. To date, many FEMs, FDMs, and spectral methods have been proposed to solve fractional PDEs. However, they suffer from heavy computational cost and memory storage, as well as other inherent shortcoming and difficulties. In this paper, a meshless method, the reproducing kernel particle methods (RKPM), is first applied to solve one kind of fractional PDE, the space fractional advection-dispersion equation that can accurately describe particle transport in complex media. Similar to FEM and FDM, the discretization matrix of RKPM is not banded due to the fractional derivative operator, which induces extensive computational cost. Based on the analysis of the fractional derivative of shape function and Taylor expansion theory, a fast approximation calculation method, referred to as the “line replacement principle” is proposed to reduce the calculation cost drastically while keeping accuracy. Additionally, an alternative method to reproduce the fractional derivation of approximation function, extension of the so-called synchronized derivative method, is studied by using a generalized Taylor series expansion. Use of a kind of meshless method offers advantages of adaptive analysis, easily treating irregular domains for solving spatial fractional PDEs.

13th U.S. National Congress on Computational Mechanics
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Title: USNCCM Symposium of High-Order Methods for Computational Fluid Dynamics

Author(s): Chunlei Liang, *George Washington U.*.

The speaker will first introduce the USNCCM series of Symposiums of High-order Methods for Computational Fluid Dynamics. The series began from 2013 held in Raleigh NC. It was organized by Professors Chunlei Liang, Krzysztof Fidkowski, Per-Olof Persson, and Peter Vincent. Subsequently, the plans of publishing a special issue for the 2015 Symposium in the Computers & Fluids journal will be discussed. This special issue will be dedicated to the 60th birthday of Professor David Kopriva. Finally, the funding from the National Science Foundation and the George Washington University will be acknowledged.

13th U.S. National Congress on Computational Mechanics
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Title: A Constitutive Model for the Thermomechanical Response of Polyurea Under Large Deformations and High Strain Rates

Author(s): Xiao Liao, Jay Oswald, *Arizona State U.*; Alireza Amirkhizi, *U. Massachusetts Lowell*.

A constitutive model is developed to model deformation and energy dissipation in polyurea coatings under cavitation erosion. As the collapse of vapor bubbles against a surface generates microscopic, yet extreme pressures, a model that combines pressure, temperature, and strain rate effects is needed to accurately characterize the material response. We have combined the pressure, temperature, and strain rate dependent viscoelastic model developed by Amirkhizi et al [1] with the stretch-dependent hyperelastic model developed by Arruda and Boyce [2] in order to represent both large strain and time-dependent response. The model is implemented with a logarithmic strain form, allowing large deformation response to be modeled in the current coordinate frame without integrability issues. Material parameters are calibrated from split-Hopkinson pressure bar tests conducted at a range of temperatures. Simulations of a cavitation bubble collapsing on polyurea coating will be presented to demonstrate the applicability of the new material model. [1] AV Amirkhizi, J Isaacs, J McGee, and S Nemat-Nasser. An experimentally-based viscoelastic constitutive model for polyurea, including pressure and temperature effects. Philosophical magazine, 86(36):5847–5866, 2006. [2] EM Arruda and MC Boyce. A three-dimensional constitutive model for the large stretch behavior of rubber elastic materials. Journal of the Mechanics and Physics of Solids, 41(2):389–412, 1993.

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Title: Multi-Scale Analysis of Macromolecular Microtubules

Author(s): Kim Meow Liew, *City U. Hong Kong*; Luwen Zhang, *Shanghai Ocean U.*.

Multi-scale Analysis of Macromolecular Microtubules ABSTRACT A computational modeling of the biomechanical behavior of microtubules based on the element-free Galerkin method and higher-order Cauchy-Born rule is carried out. A single microtubule contains up to billions of different types of atoms [1]. To analyze a microtubule, the challenge is to develop a practical theory to describe this kind of polyatomic structure with both result accuracy and computing efficiency. This work proposes a multi-scale technique based on the intrinsic interatomic potential and a continuum description method, and hence the overall mechanical performance of microtubules could be studied. The work begins with evaluation of interatomic potential using a homogenization technique; large numbers of different types of atoms are replaced by a product of volume densities and the occupied space volumes. The potential energy stored between the basic subunit of microtubules and tubulin dimmers is obtained from a mutual definite integral process between pair bodies [2]. Without tracing every single atom, deformation of macromolecules components is determined by the proposed fictitious bond connecting central points of neighboring bodies. A mesh-free theoretical and numerical framework based on a higher-order Cauchy-Born rule under the higher-order gradients continuity has been specifically constructed. This simulation scheme is generally applicable and can be employed to study the overall mechanical behavior of microtubules [3]. With the proposed methodology, elastic properties, transverse and longitudinal buckling and post-buckling behaviors, vibration modes, natural frequencies and dynamic responses are numerically simulated. References [1] K. M. Liew, P. Xiang and L. W. Zhang, Mechanical properties and characteristics of microtubules: A review. Composite Structures, 123 (2015) 98-108. [2] P. Xiang and K. M. Liew, Predicting buckling behavior of microtubules based on an atomistic-continuum model. International Journal of Solids and Structures, 48 (2011) 1730-1737. [3] P. Xiang and K. M. Liew, A computational framework for transverse compression of microtubules based on a higher-order Cauchy-Born rule. Computer Methods in Applied Mechanics and Engineering, 254 (2013) 14-30.

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Title: Simulations of Intracranial Aneurysm Flows with Active Contrast Leakage During Computed Tomography Angiography

Author(s): Ming-Lung Li, Tong-Miin Liou, Chao-An Lin, *Nat'l. Tsing Hua U.*; Yi-Chou Wang, *Chang Gung Memorial Hospital*.

Precise locations of rupture region under contrast agent leakage of five ruptured cerebral artery aneurysms during computed tomography angiography. These, together with numerical simulations based on the reconstructed aneurysmal models, were used to analyze hemodynamic parameters of aneurysms under different cardiac cyclic flow rates.

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Title: The Role of Interfacial Behavior on Extrafibrillar Matrix in Bone

Author(s): Liqiang Lin, xiaowei Zeng, Xiaodu Wang, *UTSA*.

In the hierarchy of bone, lamellae serve as the basic building unit for both human and animal bones. They are a sheet-like biocomposite of mineralized collagen fibrils embedded in an extrafibrillar matrix and dictate, to large extent, the mechanical behavior of bone. The structure and mechanical properties of mineralized collagen fibrils have been extensively studied, whereas only limited information is available regarding the role of the extrafibrillar matrix in bone mechanical behavior. In this study, we assumed that the extrafibrillar matrix consists of hydroxyapatite (HA) polycrystals that are bounded through an organic interface of non-collagenous proteins (NCPs). This organic interface may facilitate relative sliding between individual mineral crystals, thereby imparting to bone more capability of dissipating energy during bone deformation and failure process. To investigate interfacial interactions, a generalized interfacial bonding model is proposed to model the organic interface between HA crystals. The polycrystals geometrical model of extrafibrillar matrix in bone was generated using Voronoi tessellation techniques with an average crystal size 25nm. The simulation results agree well with experimental observations of bone fracture and the results indicated that this model was able to capture the following behaviors of bone as reported in experimental studies: (1) the maximum strain of mineral phase in compression modes observed in synchrotron X-ray scattering studies; (2) the sudden drop of strain in the mineral phase at the bulk yielding of bone under compression; (3) the cross-hatch damage (shear band) formation in compression; and (4) the upper bound of the in situ elastic modulus of bone.

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Title: Fast Algorithms for Electronic Structure Analysis

Author(s): Lin Lin, *UC Berkeley*.

Kohn-Sham density functional theory (KSDFT) is the most widely used electronic structure theory for molecules and condensed matter systems. For a system with N electrons, the standard method for solving KSDFT requires solving N eigenvectors for an O(N) * O(N) Kohn-Sham Hamiltonian matrix. The computational cost for such procedure is expensive and scales as O(N^3), and limits routine KSDFT calculations to hundreds of atoms. In recent years, we have developed an alternative procedure called the pole expansion and selected inversion (PEXSI) method [1-2]. The PEXSI method solves KSDFT without solving any eigenvalue and eigenvector, and directly evaluates physical quantities including electron density, energy, atomic force, density of states, and local density of states. The overall algorithm scales as at most O(N^2) for all materials including insulators, semiconductors and the difficult metallic systems. The PEXSI method can be efficiently parallelized over 10,000 - 100,000 processors on high performance machines. It has been integrated into standard electronic structure software packages such as SIESTA for ab initio materials simulation over 20,000 atoms [3]. Recently we have been able to use PEXSI to study electronic structure of large scale graphene nanoflakes [4] and phosphorene nanoribbons [5] to unprecedented scale (more than 10,000 atoms). [1] L. Lin, J. Lu, L. Ying, R. Car and W. E, Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems, Commun. Math. Sci. 7, 755, 2009 [2] L. Lin, M. Chen, C. Yang and L. He, Accelerating atomic orbital-based electronic structure calculation via pole Expansion and selected inversion, J. Phys. Condens. Matter 25, 295501, 2013 [3] L. Lin, A. Garcia, G. Huhs and C. Yang, SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization, J. Phys. Condens. Matter 26, 305503, 2014 [4] W. Hu, L. Lin, C. Yang and J. Yang, Electronic structure of large-scale graphene nanoflakes, J. Chem. Phys. 141, 214704, 2014 [5] W. Hu, L. Lin and C. Yang, Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory, accepted, Phys. Chem. Chem. Phys. 2015

13th U.S. National Congress on Computational Mechanics
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Title: Immersed Finite Element Methods with Edge Penalties for Interface Problems

Author(s): Tao Lin, *Virginia Tech*.

Interface problems often appear in numerical simulations over domains consisting of multiple materials that result in discontinuous coefficients in the involved partial differential equations whose solutions are less smooth across the material interfaces. This deficiency of the global regularity in the exact solution to interface problems requires traditional finite elements (FE) to use object-fitting meshes in which each element essentially contains one of the materials; otherwise, their convergence cannot be guaranteed. Object-fitting meshes are usually unstructured unless material interfaces have trivial geometries, and having to use unstructured meshes can negatively impact the efficiency of FE methods in some applications. The recently developed immersed finite element (IFE) methods are non-traditional FE methods that can utilize interface-independent meshes; hence, they can use structured/Cartesian meshes even for interfaces with non-trivial geometries. IFE methods use two types of shape functions: the standard polynomial FE shape functions over non-interface elements and the macro piecewise polynomial IFE shape functions on interface element elements constructed according to interface jump conditions prescribed by the interface problems. Nevertheless, with a limited degrees of freedom, the regularity of IFE functions is often lower at edges of elements than their inside. Without a suitable formulation to handle the edge discontinuity in IFE functions, an IFE method can perform unsatisfactorily, especially in its accuracy around the interface and stability. This talk will present several IFE methods with edge penalties for solving some typical interface problems. Key ingredients for the related error estimation will be discussed, and numerical examples will be provided to demonstrate features of these IFE methods.

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Title: Phase-Field Modeling of Diffusion Induced Fracture in Si Electrodes

Author(s): Christian Linder, Xiaoxuan Zhang, *Stanford U.*.

Lithium-ion batteries are important energy storage devices for portable electronics due to their high energy density and high average voltage. To improve their performance, one of the known methods is to use new electrode materials. As one of those materials, silicon (Si) is an attractive candidate with a maximum theoretical specific capacity of 4200mAh/g, compared with 372mAh/g for graphite used in current commercial Lithium-ion batteries. However, enormous volume changes (~310% at full lithiation of Si) caused by the insertion and extraction of Lithium (Li) lead to mechanical failure, chemical degradation and capacity loss of Si electrodes, and prevent Si's practical application. In the past decades, extensive research has been done to investigate the diffusion process, electrochemical reaction, stress evolution and mechanical failure for the lithiation of Si from both experimental and numerical modeling point of view. In those experiments, many interesting features for Si have been observed, such as two-phase lithiation for both crystalline Si (c-Si) and amorphous Si (a-Si), one-phase lithiation for delithiated amorphous Si (post-a-Si), diffusion induced plastic deformation and size-dependent fracture behavior. To study this complicated electro-chemo-mechanical coupled lithiation process of Si, we first propose a reaction-controlled diffusion model to describe the two-phase lithiation of c-Si and a-Si, and one-phase lithiation of post-a-Si in a consistent manner [1]. The effect of hydrostatic pressure and Li concentration level on the chemical reaction rate at the reaction front is taken into account in the new formulation. By varying the Si-Si bond-breaking barrier, representing different types of Si, both the two-phase lithiation and one-phase lithiation can be described consistently by our formulation. Next, a phase field model for fracture is coupled to this reaction-controlled diffusion model to study the lithiation induced elasto-plastic deformation and fracture in different shapes of Si electrodes at large deformation. We study the stress distribution in different electrodes. And we show that the diffusion induced anisotropic deformation in c-Si electrodes is related to the initiation of fracture. We also investigate the size effect and Li concentration on the fracture behavior of Si electrodes. Finally, we compare our numerical simulation results with existing experimental data and numerical simulation. In the future, our electro-chemo-mechanical coupled model will be used to optimize the structure of Si electrodes. [1] Zhang X, Lee SW, Lee H-W, Cui Y, Linder C, (2015). A reaction-controlled diffusion model for the lithiation of silicon in lithium-ion batteries. Extreme Mechanics Letters, submitted for publication.

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Title: Simulation of Metal Deposition of Ti-6Al-4V Using Coupled Constitutive and Microstructure Models

Author(s): Lars-Erik Lindgren, Andreas Lundbäck, *Luleå U. Tech.*; Robert Pederson, *GKN Aerospace Eng. Sys.*.

The main challenges for additive manufacturing (AM) is to achieve near net shape with high quality material properties. The latter includes optimal microstructure and low residual stresses. This quality is of particular important in aerospace applications and therefore accurate models are needed. Simulation of a validation case of additive manufacturing for Ti-6Al-4V is demonstrated in the presentation. The TIG process is used to deposit a wire on a plate in a complex pattern. Temperatures and deformations are measured and compared with calculated results. The focus of the paper is on the plasticity [1] and phase change models [2]. A dislocation density based plasticity model is used. It includes a long-range term, typically called strain hardening, as well as a short-range term with an explicit rate and temperature dependency. The alfa-beta phase changes are calculated using a JMAK type of model. The numerical technique used for imitating the addition of material in the AM process is similar to what has been used in simulation of multipass welding. However, there are additional complications mainly due to the large amount of added material and possibly large deformations. This is also discussed in the presentation. Acknowledgments Funding via the strategic innovation programme LIGHTer as well as from the Swedish National Space Research Program, provided by Vinnova in both cases, are acknowledged. References 1. Babu, B. and L.-E. Lindgren, Dislocation density based model for plastic deformation and globularisation of Ti-6Al-4V. International Journal of Plasticity, 2013. 50: p. 94-108. 2. Charles Murgau, C., R. Pederson, and L.-E. Lindgren, A model for Ti-ì6Al-ì4V microstructure evolution for arbitrary temperature changes. Modelling and Simulation in Materials Science and Engineering, 2012. 20(5): p. 055006.

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Title: PreCICE - A Flexible and Versatile Coupling Library

Author(s): Florian Lindner, Miriam Mehl, *U. Stuttgart*; Benjamin Uekermann, *Techn'l. U. Munich*.

Flexible and extensible partitioned multi-physics simulation environments require efficient and modular tools with a broad coupling functionality. preCICE is a library for flexible numerical coupling of single-physics solvers. It uses a partitioned black-box coupling scheme, thus requiring only minimal modifications to existing solvers. Codes currently coupled with preCICE comprise both commercial and academic solvers, with a particular focus on fluid-structure interaction. preCICE features a clean and modern software design with extensive unit and integration testing. Inter-solver parallelism, parallel communication and data mapping techniques help to scale even on exascale machines.

13th U.S. National Congress on Computational Mechanics
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Title: Cohesive Dynamics and Fracture

Author(s): Robert Lipton, *Louisiana State U.*.

Dynamic brittle fracture is a multiscale phenomena operating across a wide range of length and time scales. Apply enough stress or strain to a sample of brittle material and one eventually snaps bonds at the atomistic scale leading to fracture of the macroscopic specimen. In this talk we formulate a nonlocal, multi-scale, cohesive continuum model for assessing the deformation state inside a cracking body. This model is expressed using the peridynamic formulation introduced in [2]. We choose a peridynamic model for which the short-range forces between material points are unstable and soften beyond a critical relative displacement. The nonlinear elastic–softening behavior is similar to the ones use in cohesive zone models introduced by Dugdale and Barenblatt. In this model the dynamics selects whether a material point lies inside or outside the process zone associated with nonlinear behavior. The evolution of the process zone now becomes an intrinsic feature of the dynamics. This is in contrast to classic cohesive zone models that collapse the process zone onto lower dimensional sets constrained to lie on prescribed surfaces. In this formulation the natural length scale that controls the size of the process zone is the radius ε of the horizon of interaction between particles. We derive an explicit inequality that shows that the size of the process zone is controlled by the horizon radius. Points within the process zone are shown to provide nucleation sites for fracture initiation. The volume of the process zone is shown to go to zero with ε and collapses onto a set of lower dimension in the limit of vanishing non-locality, $\varepsilon \to 0$. In this limit it is seen that these models have a process zone that conforms to the assumptions of Linear Elastic Fracture Mechanics. Distinguished $\varepsilon \to 0$ limits of cohesive evolutions are identified and are found to have both bounded linear elastic energy and Griffith surface energy. The limit dynamics corresponds to the simultaneous evolution of linear elastic displacement and a fracture set across which the displacement is discontinuous. These results are reported in [1]. References. [1]. R. Lipton. Cohesive Dynamics and Fracture. arXiv:1411.4609v3 [math.AP] 11 Dec 2014. [2]. S.A. Silling. Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces. J. Mech. Phys. Solids 48 (2000) 175-209.

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Title: Modeling Damage and Thermal Effects in Composite Materials Using an Enrichment Based Multi-Scale Method

Author(s): Michael Macri, *Benet Labs*; Andrew Littlefield, *US Army Benet Labs*.

The defense industry is increasingly incorporating composite materials into military systems, many of which undergo rapid and severe changes in temperature, as well as subject the composites to physical trauma or environmental conditions that can cause micro damage leading to variations of the mechanical properties. For these applications, it is crucial to develop models that can accurately simulate the response of these materials. Damage on the micro-structure of composites, such as micro-cracks, fracture, debonding and voids, can have a significant effect the global response of the system. Though empirical data can be used to approximate the material properties for an ideal non-damaged specimen, performing experimentation on damaged composites and extracting a correlation between micro-crack size and/or quantity to material properties can be extremely difficult. One approach to extract material properties from a composite material without having to perform experimental testing is a numerical approximation method, called the homogenization method. A limitation with the homogenization method is that it suffers from a basic assumption that there is uniformity of the macroscopic fields within each representative volume element (RVE). Hence, this method breaks down in critical regions of high gradients such as cracks. This further complicates its use for modeling micro-crack phenomena, as it is in regions of macro-cracks that micro-cracking will be formed. For this presentation, we will demonstrate the use of a structural based enrichment method to accommodate micro-cracking. This approach can be used in regions where macro-cracks are assumed to have initiated. The structural based enrichment method is based on the principles of partition of unity, which allows enrichment of the approximation space in localized sub domains using specialized functions that may be generated based on a priori information regarding asymptotic expansions of local stress fields and microstructure. The research presented reviews the derivation of the enrichment functions needed to represent the micro-structure, which is a piece-wise numerical representation of the micro-displacement to macro-strain relationship. Because of the piece-wise nature of the function, it is dependent on the geometry of the micro-structure, enabling it to contain various levels of micro-cracks. The research demonstrated that using the enrichment functions improved solutions by reducing the error up to 15%.

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Title: Coupling Approaches for Integrating Meshfree Peridynamic Models with Classical Finite Element Analysis

Author(s): David Littlewood, Stewart Silling, John Mitchell, *Sandia Nat'l. Lab.*; Pablo Seleson, *Oak Ridge Nat'l. Lab.*.

The meshfree discretization of peridynamics first proposed by Silling and Askari enables large-scale simulations of material damage and failure. Its use in complex, system-level analyses is restricted, however, due to several considerations. Peridynamics is more computationally expensive than classical finite element (FE) approaches, requires nonlocal volumetric constrains that may be difficult to apply in practice, and does not currently support the broad set of features commonly found in mainstream FE codes, such as structural elements. Combined analyses in which peridynamics is employed only in regions susceptible to material failure are therefore highly desirable, yet approaches for model coupling remain limited. We present strategies for coupling meshfree peridynamic models with FE implementations of classical continuum mechanics. The challenges associated with coupling local and nonlocal formulations are first addressed at the continuum level, where the finite length scale associated with peridynamics leads to an incompatibility with classical models. A novel peridynamic formulation that supports a variable horizon mitigates this incompatibility by allowing the nonlocal length scale to be reduced in the direct vicinity of a model interface. Model coupling is further enhanced through the use of a blending scheme that addresses the so-called ghost forces observed at boundaries between local and nonlocal models. The coupling approaches are demonstrated in the open-source peridynamics code Peridigm and the classical finite-element code Albany.

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Title: Non-Invasive, In-Vivo Quantification of Mechanical Heterogeneity of Invasive Breast Carcinomas

Author(s): Tengxiao Liu, Assad Oberai, *RPI*; Olalekan Babaniyi, Paul Barbone, *Boston U.*; Timothy Hall, *U. Wisconsin*.

In gross pathology, cancerous tumors appear to be heterogeneous and have rough margins. This is because of the desmoplastic reaction which is usually only associated with malignant tumors. Desmoplasia is characterized by the pervasive growth of dense collagen fibers. More collagen fibers imply higher elastic modulus. Therefore it is reasonable to expect that malignant tumors would appear as heterogeneous masses in elastic modulus images. In this study we develop a novel method to quantify the mechanical heterogeneity within malignant and benign tumors using ultrasound based elasticity imaging. Using free-hand ultrasound-based elasticity imaging, data was acquired on a set of ten patients: five with a fibroadenoma (FA) and five with invasive ductal carcinoma (IDC). The ultrasound radiofrequency echo data was used to determine displacement field within the breast at a resolution of about 200 microns. This displacement field was used in an inverse algorithm to determine the spatial distribution of the Young's modulus at the same resolution. Thereafter a heterogeneity parameter (denoted by H), which is roughly the ratio of the tumor size to the correlation length of the modulus distribution within the tumor, was evaluated for each tumor. It was found that the value of this parameter was higher for cancerous tumors. By using $H > 0.6$ as a criterion for malignancy, an accuracy of 90% (100% sensitivity and 80% specificity) was attained. Our results verify that malignant lesions are mechanically more heterogeneous than benign lesions through high-resolution quasi-static elasticity imaging. They also demonstrate that mechanical heterogeneity may be used to improve the specificity of breast ultrasound imaging.

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Title: Multi-Scale Analyses of Wave Propagation in Heterogeneous Media

Author(s): Chenchen Liu, Celia Reina, *U. Pennsylvania*.

In this talk we present an efficient multiscale model for the study of the dynamic behavior of heterogeneous media in the spirit of multiscale finite element method FE2. This new computational strategy is exemplified for the case of wave propagation in periodic microstructure for different frequencies and microstructural details. Comparisons with solutions attendant to a standard finite element analyses indicate that the model is capable of accurately capturing the dispersion in the media.

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Title: Weighted T-Spline and its Application in Isogeometric Analysis

Author(s): Lei Liu, Yongjie Zhang, *Carnegie Mellon U.*.

To facilitate isogeometric analysis, we present a new type of T-spline named weighted T-spline, which introduces a weighting idea to T-spline basis functions. Weighted T-spline basis functions satisfy partition of unity and are linearly independent. To handle extraordinary nodes, the knot intervals are constrained to be the same within their two-ring neighborhood. The surface continuity is C2 everywhere except edges shared by the one-ring neighborhood elements, which is C0 continuous. Compared to standard T-splines, the weighted T-spline has less geometrical constraints to the T-mesh, and can decrease the number of control points significantly, especially in 3D situations. We apply the weighted T-spline to volumetric T-spline construction from B-reps of designed CAD models. The weighted T-spline is first used to reparameterize trimmed NURBS surface patches. Edge interval extension is performed to reconstruct the trimming curve on the T-spline surface, and the trimming curve can be exactly reconstructed. The surface error introduced by weighted T-spline basis functions is bounded (e.g., within 1%) and the error introduced by the trimming curve is constraint within its three-ring neighboring elements. Then the reparameterized T-spline surfaces are combined together to generate water-tight weighted T-spline surfaces, with extraordinary nodes properly introduced. The T-spline surfaces are further converted to volumetric weighted T-spline using the polycube method. Finally Bézier elements are extracted from the generated weighted T-spline models for analysis. Weighted T-spline models are applied to solving linearly elasticity problems and Poisson's equations, demonstrating that they are analysis-suitable.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Modeling Laminated Composites via a Novel Nonlocal Lattice Particle Framework

Author(s): Hailong Chen, Yongming Liu, *Arizona State U.*.

A nonlocal lattice particle framework, the Volume-Compensated Particle Model (VCPM), was applied to model the elastic and fracture response of laminated composites. In VCPM, the domain of interest is decomposed into particles which are located at lattice sites according to various packing format, e.g., triangular packing in 2D and simple cubic packing in 3D. The VCPM particles are connected via linear springs and the interaction between a typical particle pair not only has contribution from the connecting spring itself, but also affected by all its neighbors. Comparing to other continuum based models, such as FEM, VCPM is a discrete bond based model and has many advantages for fracture modeling over other numerical methods. Crack initiation and propagation is the natural outcome of bond breakage, and no external crack propagation criteria are required. Distinct from the bond based Peridynamics, there is no limitation on the materials' Poisson's ratio, i.e., materials with arbitrary Poisson's ratio can be modeled within the proposed framework. Besides, the ply orientation is represented by rotating the underlying particle structure, rather than transforming the material stiffness matrix which is generally used in current numerical methods. By employing this scheme, not only the material but also the geometric orthotropy both are considered in this proposed framework. This is considered as one of the most prosperous property of this model. The simulated results are verified with both analytical solutions and experimental observations and good agreements are found.

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Title: A Face-Based/Node-Based Selective Smoothed Finite Element Method (FS/NS-FEM) for Cardiovascular Tissues Using Linear Tetrahedral Elements

Author(s): Chen Jiang, *Hunan U.*; G.R. Liu, *U. Cincinnati*.

Cardiovascular diseases (CVD) have the leading death rate globally, and are often caused by lesions of heart and blood vessel, Like Abdominal Aortic Aneurysm and cardiac hypertrophy. Hence, organs which are originally with complex geometry in cardiovascular system become much more complex in geometry. To analyze the mechanical responses of a complex geometry using FEM, a fully hexahedral mesh is preferred, but often difficult and laborious even impossible to be generated. Tetrahedral elements (T4) are on the other hand much more easier to generated, and can even done automatically. The existing programs are quite robust and can automatically create tetrahedral mesh efficiently for complicated geometries. The remaining concerns of using tetrahedral elements are the inaccuracy and the locking phenomena of linear tetrahedron. Therefore, to find an accurate, efficient, robust and locking free tetrahedral algorithm using T4 elements is what many researchers have been pursuing for years. To achieve this goal, we incorporated the strain smoothing techniques with FEM to create a new family of the so-called Smoothed Finite Element Method (S-FEM). Different strain smoothing techniques give T4 elements in S-FEM with quite different properties. For nearly-incompressible cardiovascular tissues, selectively using the face-based S-FEM (FS-FEM) for the deviatoric deformation and the node-based S-FEM (NS-FEM) for the volumetric deformation is a simple, effective and accurate way to handle the volume locking. A benchmark test calculating a thick sphere with internal pressure shows that the FS/NS-FEM-T4 has remarkable robustness against element distortion. It has the similar efficiency as the FEM-T10-SRI, and no volumetric locking for nearly- incompressible materials. The FS/NS-FEM-T4 is also used to calculate a MRI-based human Abdominal Aortic Aneurysm (AAA) with systolic blood pressure and a rabbit ventricle in diastole. The close stress distributions with FEM-T10-SRI and agreed results with experiments of both examples demonstrate FS/NS-FEM has greatly improved the accuracy, efficiency and robustness of T4 elements for complicated geometries.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling Acoustic Metamaterials Using the Boundary Element Method

Author(s): Anli Wang, Yijun Liu, *U. Cincinnati*; Bangjian He, *NW Polytech. U.*.

In this talk, we report some preliminary results of modeling acoustic metamaterials using the boundary element method (BEM). Specifically, we have applied the 2-D and 3-D BEM for solving acoustic wave problems to model phononic crystal structures to detect the band gap phenomenon. We assumed that arrays of rigid and long cylinders are placed in the air and impinged upon by an incident wave. The sound fields on the other side of the arrays are computed at different frequencies using both the 2-D and 3-D BEM programs that are accelerated by the fast multipole methods. The results show clearly the band gaps for the models used which are also consistent with the data reported in the literature. This preliminary study shows the potential of using the fast multipole BEM in the research on acoustic metamaterials. Some related computational issues in using the BEM will also be discussed during this talk.

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Title: Wave Propagation Analysis for 3D Non-Homogeneous Materials by Using Time-Domain BEM Based on RIM

Author(s): Liqi Liu, Haitao Wang, *Tsinghua U.*; Chenfeng Li, *Swansea U.*.

The boundary element method (BEM) has been widely used to simulate the soil in dynamic Soil-Structure Interaction (SSI) analysis. The properties of the soil may have a significant effect on the wave propagation process. Studies in the literatures on dynamic SSI analysis are mainly limited to homogeneous and layered homogeneous domains. These simplified assumptions might lead to considerable errors in practical geotechnical problems since soils generally exhibit non-homogeneous behaviour because of their natural sedimentation process. An efficient way to improve the accuracy is to treat the soil as continuously non-homogeneous material of which the properties vary with position. In geotechnical engineering, the non-homogeneity of soil deposits is often described by the increase of elasticity modulus and density as a power function of depth. Despite of the extended literatures on dynamic problems of homogeneous and layered homogeneous domain, few works are found for analysing transient response of continuously nonhomogeneous body in time domain. The main reason behind this is the challenge of generating appropriate fundamental solutions for this type of problems. The conventional 3D dynamic fundamental solutions are derived based on isotropic homogeneous domain, and cannot be applied to non-homogeneous problems directly. An alternative approach is the application of static fundamental solutions. In this case, domain integrals resulted from the inertial term as well as the non-homogeneity are included in the boundary-domain integration equations (BDIEs). Conventionally, domain discretization is required to evaluate these domain integrals. Although cell integration scheme can give accurate results, the discretization of domain into cells may offset the main advantage of BEM that only boundary discretization is needed. In order to avoid domain discretization, various techniques have been developed to transform these domain integrals into boundary integrals, for example, dual reciprocity method (DRM) and radial integration method (RIM). In the present paper, to solve the 3-D elastodynamic problem with non-homogenous domain, the conventional fundamental solutions for 3D, linear elastic, isotropic, homogeneous problems are employed to form the boundary-domain integration equations and the RIM is implemented to transform the arising domain integrals into boundary integrals. After boundary discretization is carried out, a set of second-order ordinary differential equations with respect to time variable similar to that provided by the finite element method (FEM) are derived. These equations are solved using several different time-stepping algorithms, which are compared in terms of accuracy and stability.

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Title: Boiling Flows: Thermomechanical Theory, Entropy-Stable Algorithm, and Simulations

Author(s): Ju Liu, Chad Landis, Thomas Hughes, *UT Austin*; Hector Gomez, *U. A Coruna*.

Boiling flows are widely used as an energy transfer mechanism in practice. However, due to its disparity of spatiotemporal scales and elusive nature of many sub-processes, a complete theory of boiling is still lacking. Current studies on phase-field models mainly focus on bubble dynamics and free surface problems. The full capability of phase-field type multiphase models has not been fully realized by the multiphase flow community. In this work, we first systematically derive a new modeling framework for multiphase flows, using the celebrated microforce theory developed by Gurtin [1]. This modeling framework guarantees entropy production intrinsically. We will show that the thermomechanical theory derived by Dunn and Serrin is a special case in this framework by choosing an appropriate thermodynamic potential function. A new fully discrete scheme is constructed to solve the aforementioned thermomechanical theory, i.e., the Navier-Stokes-Korteweg equations [3]. In particular, the spatial discretization is designed based on the notion of functional entropy variables. A new time integration scheme is constructed based on a family of novel quadrature rules. The resulting fully discrete scheme is provably entropy dissipative and second-order accurate in time. In the presence of complex geometries and high-order differential terms, isogeometric analysis [2] is invoked to provide accurate representations of computational geometries and robust numerical tools. The pool boiling problem is numerically investigated by making proper assumptions on transport parameters and boundary conditions. Compared with traditional multiphase solvers, the dependency on empirical data is significantly reduced for boiling simulations. It will be demonstrated that this modeling approach provides a unified predictive tool for both nucleate and film boiling. Both two and three-dimensional simulation results will be provided and discussed. References [1] M.E. Gurtin. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a micro force balance. Physica D: Nonlinear Phenomena, 92:178–192, 1996. [2] T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry, and mesh refinement. Computer Methods in Applied Mechanics and Engineering, 194:4135–4195, 2005. [3] Ju Liu. Thermodynamically Consistent Modeling and Simulation of Multiphase Flows. PhD thesis, The University of Texas at Austin, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: Consistent Time Integration for Dynamics Across Numerical Interfaces Between Geometrically Exact Beams and Continuum Finite Elements

Author(s): Hui Liu, Arun Prakash, *Purdue U.*.

Geometrically exact beam models are widely used in simulations of structures undergo large deformations. However, beam models are limited in their ability to capture realistic behavior at structural joints especially under large deformations and/or damage. On the other hand, high-fidelity continuum models are able to simulate more realistic behavior, but the computational cost associated with these types of models grows rapidly with problem size and thus makes it impractical to use in large-scale simulations. In the current study, a spatial domain decomposition approach is used which permits one to decompose the structure into ‘critical’ and ‘non-critical’ regions. The ‘critical’ regions can be simulated using detailed continuum models while the ‘non-critical’ regions are simulated using computationally efficient beam models. In this way, detailed realistic behavior of the critical regions can be captured while still maintaining a low overall computational cost. This spatial domain decomposition approach creates the need for devising effective coupling of beam and continuum elements at the interface between the ‘critical’ and ‘non-critical’ regions. A geometrically consistent method for coupling beam and continuum finite elements that accounts for large deformations and large rotations is developed. The key idea is to impose the geometric constraint of rigid sections, that forms the basis of beam theory, onto the interface between the beam and continuum regions in a mathematically consistent manner. In addition to spatial domain decomposition, different temporal scales are also adopted for beam and continuum regions to improve the computational efficiency for dynamic problems. Using the energy-momentum method as a basis, a multi-time-step method for dynamic coupling of beam-continuum models is developed in the current study. Several numerical examples are presented to characterize the performance of this approach with respect to stability, accuracy and computational cost.

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Title: A Robust Nitsche's Formulation for Interface Problems with Application to the Surfactant-Driven Fracture of Particle Rafts

Author(s): Yingjie Liu, John Dolbow, *Duke U.*; Mahesh Bandi, Eliot Fried, *Okinawa Inst. Sci. & Tech.*.

This study presents a robust Nitsche's method to model static and evolving interface problems with embedded finite element techniques. With embedded methods, an important consideration is the need for modified quadrature schemes to accurately integrate partial elements. Since the geometry of the partial element can be complicated, submeshing is usually employed. In this talk, we propose an alternative technique that does not require submeshing and greatly improves efficiency. We also address the issue of determining the stabilization parameter in Nitsche's method. A general approach is proposed to estimate the stability parameter for non-constant strain elements. The method is then used to approximate the solution to benchmark elliptic interface problems. The results are compared to those obtained with immersed interface methods and other popular algorithms for embedded interface problems. Our method is further extended to model the surfactant-driven fracture of particulate rafts [1-2]. A significant challenge for simulations of this system is that the movement of particles leads to rapid changes in the geometry of the computational domain. The proposed method treats the particles as rigid bodies that interact through an attractive force in a discrete particle dynamics approach. Their coupling to surfactant diffusion is then effected via the embedded finite element method. Our simulations successfully reproduce the experimentally observed process whereby surfactant transport drives particles into a jammed band that gradually splits into periodically arranged triangular sectors. [1] D. Vella, H.-Y. Kim, P. Aussillous, and L. Mahadevan, 2006. Dynamics of Surfactant- Driven Fracture of Particle Rafts. Physical Review Letters. 96, 178301. [2] M. M. Bandi, T. Tallinen and L. Mahadevan, 2011. Shock-driven jamming and periodic fracture of particulate rafts. European Physics Letters, 96, 36008.

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Title: Pattern Characterization and Volume-Integral Micromechanics Model of Elastic and Elastoplastic Heterogeneous Material

Author(s): Zeliang Liu, Wing Kam Liu, *Northwestern U.*.

A continuing challenge in computational material design is developing a multiscale model to link the microstructure of a material to its material properties at a larger length scale in both an accurate and computationally efficient manner. In our work, such a model is developed which uses the statistical descriptors of the microstructure combined with a pattern-based volume-integral micromechanics (PVM) model. Rather than solving the whole material domain in DNS methods like FEM and FFT-based method, PVM characterizes the microstructures into different patterns through imaging processing techniques, and then use volume integral equation to solve the effective stress/strain in each pattern self-consistently. Since the number of defined patterns is much less than the number of degrees of freedom in DNS, PVM is more efficient than DNS method. At the same time, it keeps more field information (e.g., stress concentration) than traditional micromechanics models, such as Mori-Tanaka and self-consistent methods. The model is applied to elastic and elastoplastic heterogeneous material with arbitrary phase geometry. For both 2D and 3D problems, PVM's capability of predicting the effective properties at the macroscale is validated against experiments and FEM simulations. Moreover, PVM can be further extended to failure in heterogeneous material. A basic framework of the material characterization and property prediction is proposed in this work. The original images are firstly characterized to provide geometric patterns and statistical descriptors, including volume fractions and the distribution of each patterns. For pattern characterization, the interaction intensity of each microstructure is determined by a Green-function-based processing method. According to the interaction intensity, all possible microstructures are classified into a reduced set of patterns, so that the new calculation is more efficient. By performing the volume integral of Green's function in each pattern, the self- and pair-interaction matrices can be determined based on whether the integration points is inside or outside the pattern. Then all the descriptors are put into a self-consistent equation which considers both self- and pair-interactions. By solving the self-consistent equation, ensemble averaged strain in each pattern are obtained. The effective properties can be calculated by averaging among all the patterns weighted by their volume fractions. For elastoplastic material, the material law is applied to each pattern. Plastic strain in each pattern are superimposed to the original elastic strain field, and the influence of plastic strain is determined by the self- and pair-interaction matrices. Keywords: multi-scale modeling, pattern characterization, statistical descriptors, volume integral, elastoplasticity

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Title: A Non-Local, Multi-Scale Discrete-Continuum Model for Granular Materials

Author(s): Yang Liu, WaiChing Sun, Zifeng Yuan, Jacob Fish, *Columbia U.*.

A three-dimensional nonlocal multiscale discrete-continuum model has been developed for modeling mechanical behavior of granular materials. In the proposed multiscale scheme, we establish an information-passing coupling between the discrete element method (DEM), which explicitly replicates granular motion of individual particles, and a finite element continuum model, which captures nonlocal overall response of the granular assemblies. The resulting multiscale discrete-continuum coupling method retains the simplicity and efficiency of a continuum-based finite element model while circumventing mesh pathology in the post-bifurcation regime by means of staggered nonlocal operator. We demonstrate that the multiscale coupling scheme is able to capture the plastic dilatancy and pressure-sensitive frictional responses commonly observed inside dilatant shear bands, without employing a phenomenological plasticity model at a macroscopic level. In addition, internal variables, such as plastic dilatancy and plastic flow direction, are now inferred directly from granular physics, without introducing unnecessary empirical relations and phenomenology. The model is used for predicting the dynamic and quasi-static responses of granular materials. The simple shear and the biaxial compression tests are used to analyze the onset and evolution of shear bands in granular materials and sensitivity to mesh density. The robustness and accuracy of the proposed multiscale model are verified in comparisons with single-scale benchmark DEM simulations.

13th U.S. National Congress on Computational Mechanics
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Title: Experimentally Consistent Process Modeling Techniques for Additive Manufacturing Methods

Author(s): Jacob Smith, Jian Cao, Wing Kam Liu, *Northwestern U.*.

Additive manufacturing (AM) methods are used for creating complex 3D geometries by depositing material particles on a substrate and imparting a high intensity heat source, e.g., lasers and electron beams, on those particles in order to fuse them together into a solid component. These methods have risen to be one of the top priorities in engineering research in the last few years and the primary reasons behind the rapid ascension of this topic in the research community include: (1) the ability to create complex geometries which are otherwise unmanufacturable by traditional manufacturing methods, (2) increased freedom on material composition and materials design through adjustment of the ratios of the composing powders, and (3) extremely fast production of new parts due to a lack of need for additional tooling and dies. However, the highly localized and intense nature of these processes elicits many experimental challenges which ultimately motivate a strong need for computational investigation of the process. The present work will discuss these challenges and methods for creating experimentally consistent macroscale process models and their impact on multiscaling to study subscale material behavior. The primary focus of this work is on best practices in thermal analysis of the process as this is the primary driver dictating the final product performance through the melting and solidification behavior/cooling rate, which control the microstructure and phase composition, and thermal gradients, which affect the microstructure and residual stresses.

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Title: Enhanced Element Deletion Method and Applications in the Modeling of Fracking

Author(s): Zhanli Liu, Tao Wang, Zhuo Zhuang, *Tsinghua U.*; Haiyan Li, *China Acad. Aerospace Aerodynamics*.

In this paper a three dimensional enhanced element deletion method (EEDM) is developed by incorporating the advantages of level set method and cohesive elements to deal with the modeling of fracking in heterogeneous and layered rocks. Comparing with the traditional element deletion method, EEDM can easily capture the fracture front by level set function and get a relatively accurate crack tip field by nonlocal averaging of the stress and strain fields. Specially, fluid pressure can be easily applied on the crack surface and the continuity of fracture surface is guaranteed which was a tough nut in the modeling of three dimensional fracture propagation. On the other hand, cohesive element is combined with the element deletion method to model the weak zone like contacts, joints, faults in the rocks. So a hydrofracture can propagate, deflect, arrest or penetrate the weak zone. Fracture branching and the multi-fractures caused by material inhomogeneity are simulated to show the applicability and accuracy of EEDM. At last, the propagation of hydraulic fracture in the layered rocks is modeled and the dependence of the crack deflection, arrest, going along interfaces or penetration on the mechanical properties of the interface is studied.

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Title: Non-technical Presentations in Memory of Ted Belytschko

Author(s): W.K. Liu, *Northwestern U.* ; J.T. Oden, T.J.R. Hughes, *UT Austin*; E. Ramm, *U. Stuttgart*; S. Nemat-Nasser, J.S. Chen, *UCSD*; P. Ladeveze, *LMT-Cachan*; E. Onate, *CIMNE*; C. Farhat, *Stanford U.*; R. de Borst, *U. Glasgow*; J. Fish, *Columbia U.*.

The session will contain non-technical presentations given in memory of Professor Ted Belytschko.

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Title: Direct Numerical Simulation of Shock-Wavy-Wall Interaction by High-Order Spectral Difference Methods

Author(s): Guido Lodato, *Normandie U., CNRS, INSA U. Rouen* ; Luc Vervisch, *Normandie U., CNRS, INSA U. Rouen*; Paul Clavin, *Aix Marseille U., CNRS*.

Based on an experiment of shock reflexion on a wavy wall recently performed in a shock tube by the group at IUSTI Marseille, the present study focuses on the Direct Numerical Simulation (DNS) of an identical setup using a high-order Spectral Difference [1] code originally developed at Stanford by A. Jameson's group. Shock capturing capabilities are obtained through a Laplacian diffusion term triggered by a highly selective spectral sensor, based on the modal decomposition of the density via orthogonal polynomials [2]. The method is here slightly modified by the addition of an auto-calibration algorithm for the shock-sensor parameters. Regarding the configuration under study, in particular, the relatively complex flow structures generated by the incident planar shock (Mach 1.5) reflected by a wavy wall having a one dimensional sinusoidal shape are thoroughly analyzed. Immediately after reflection, a strongly cusped and periodic cell structure with crests (cusps) pointing toward the concave part of the wavy wall are observed on the reflected shock front. Later on these cusps split into triple points, propagating in opposite directions along the quasi-planar shock front, whose trajectories form a diamond-shaped pattern of increasing complexity. To better understand the details of such a complex flow topology, a DNS over 1.35M degrees of freedom was performed. Qualitative and quantitative validation against the available experimental data are presented and excellent agreement between the experiment and the simulation is observed. The nature of the transverse waves, which originate at the triple points on the reflected shock, is thoroughly investigated. The relevant analysis reveals that these transverse wave fronts, which are clearly responsible for the formation of the diamond shaped flow structures which are observed in the shocked region of the reflected shock, are sonic waves propagating at about the speed of sound and periodically interact with each other by subsequent collisions. Each collision gives origin to one cusp per wave front and to the formation of the observed diamond-like pattern. An investigation of the flow topology in the shocked region is carried out by the analysis of the instantaneous streamline patterns and the relevant critical points. Additionally, the results of a modeled equation describing the dynamics of the shock interface [3] are compared against the simulations. [1] Sun, Wang, Liu 2007. Commun.Comput.Phys. 2(2). [2] Persson, Peraire 2006. AIAA P. 2006-112. [3] Clavin 2013. J.Fluid.Mech. 721.

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Title: WebCL-Based Online Medical Image Segmentation with Graph Spanners

Author(s): Alex Loney, Sinan Kockara, tansel halic, *U. Central Arkansas*.

The medical imaging and image processing techniques, ranging from microscopic to macroscopic, has become one of the main components of diagnostic procedures to assist physicians in their medical decision-making processes. Computer-aided image segmentation for medical images is one of the core components of diagnostic procedures and therapeutic interventions. In this study, we introduce a web based parallel image segmentation algorithm which is implemented with WebCL. Our algorithm is based on graph spanners in which high level patterns represented in an image are exposed by a graph spanner. As a testbed we used dermoscopy images. The results demonstrate that our approach finds both the lesions and the lesion borders in dermoscopy images with high accuracy rates. Moreover, speed-up of over 30-fold over serial implementation is achieved with the parallel WebCL version.

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Title: Non-Linear Stabilization of High-Order Schemes in Unstructured Grids via Local Fourier Spectral Filtering

Author(s): Manuel López-Morales, Antony Jameson, *Stanford U.*.

One of the main barriers to wide adoption of high-order numerical methods in industrial applications is the schemes' low robustness relative to low-order methods. HiFiLES, an open-source, high-order, Navier-Stokes solver for unstructured grids is not impervious to this problem. Its stability is generally highly dependent on the quality of the grid. This presentation describes possible extensions of the LFS filters from the original tensor-product formulation to a general high-order polygon or polyhedron, with special attention to the Flux Reconstruction (FR) approach used in HiFiLES. LFS filters are uniquely suited to implementation in highly-parallelizable numerical schemes like FR because they operate element-wise, use interface information that is already used by the element to advance the solution, are provably-stable for non-linear fluxes (given enough grid refinement), and maintain the operational complexity of the underlying scheme (the filtering operation is one matrix multiplication). The presentation starts by showing the formulation of LFS filters and theoretical results regarding its stability in non-linear PDEs in one dimension. In this section, it is explained how the information from surrounding elements is used to smoothen the solution in the element being filtered. The filtering occurs by multiplying a vector containing the conservative solution and the element's adjacent conservative solution by a pre-computed matrix. This matrix is found via convolution of the basis function at each solution point with a filtering kernel. The presentation then proceeds to describe extensions proposed by Asthana et al. to two and three-dimensional tensor product elements. Once the challeneges of extensions to non-tensor product elements (triangles, tetrahedra, prisms, and pyramids) become aparent, the presentation shows our proposed general filter formulation. The properties of this filter are described. In essence, the proposed formulation gathers information from neighboring elements and stores them in a vector together with the element's conservative solution. This vector is left-multiplied by a rectangular matrix. The entries acting on the conservative solution values are pre-computed via convolution. The entries acting on the neighboring conservative solution values are found via radial functions. These entries scale the influence of neighboring elements on the filtered element's solution. The presentation ends by showing two and three-dimensional simulations that would not be possible without filtering: transonic NACA 0012 airfoil (2D) and high-Re flow over a SD7003 wing section.

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Title: An Optimization-Based Approach to Stiffness and Strength Degradation Models

Author(s): Zahra S. Lotfian, *U. Buffalo*.

A novel approach is presented for incremental state update in material models with stiffness and strength degradation. The method is based on casting the computation in each time increment as a mathematical program which includes a large class of problems related to optimization. This is an alternate method to the classical displacement-based methods where in each time increment of a numerical solution, the state of a model is computed in a nested fashion. In the optimization-based approach, the material model is fully described by specifying two scalar-valued functions – a stored energy function and a dissipation function. Once these two functions are constructed, differential equations for the evolution of the kinematic variables are obtained using the derivatives of the stored energy and dissipation functions. The optimization problem is then achieved by discretizing these equations in time.

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Title: Modelling and Simulation of Metal Deposition on a Ti-6al-4v Plate

Author(s): Andreas Lundbäck, Lars-Erik Lindgren, *Luleå U. Tech.*; Robert Pederson, Magnus Hörnqvist, Almir Heralic, *GKN Aerospace Engine Sys.*; Craig Brice, *NASA* ; Axel Steuwer, *MAX VI Lab.*; Thomas Buslaps, *European Synchrotron Radiation Facility* .

There are many challenges in producing aerospace components by metal deposition (MD). One of them is to keep the residual stresses and deformations to a minimum. Anotherone is to achieve the desired material properties in the final component. A computer model can be of great assistance when trying to reduce the negative effects of the manufacturing process. In this work a finite element model is used to predict the thermo-mechanical response during the MD-process. This work features a pysically based plasticity model coupled with a microstructure evolution model for the titanium alloy Ti-6Al-4V. A thermally driven microstructure model is used to derive the evolution of the non-equilibrium compositions of α-phases and β-phase. Addition of material is done by activation of elements. The method is taking large deformations into consideration and adjusts the shape and position of the activated elements. This is particularilly important when adding material onto thin and flexible structures. The FE-model can be used to evaluate the effect of different welding sequenses. Validation of the model is performed by comparing measured deformations, strains, residual stresses and temperatures with the computed result. The deformations, strains and temepratures are measured during the process. The deformations are measured with a LVDT-gauge at one location. The strains are measured with a strain gauge at the same location as the deformations. The temperature is measured at five locations, close to the weld and with an increasing distance of one millimeter between each thermo couple. The residual stresses in MD component were measured non-destructively using high-energy synchrotron X-ray diffraction on beam line ID15A at the ESRF, Grenoble.

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Title: Understanding Hip Fracture by Image-Based, Two-Level Biomechanical Modelling

Author(s): Yunhua Luo, Masoud Nasirisarvi, *U. Manitoba*.

Introduction Low-trauma hip fracture has become a major health problem among old people over the world, mainly due to population aging and the prevalence of osteoporosis. Sideways fall is the most critical situation for old people to develop hip fracture. However, whether or not a fall would actually result in hip fracture is determined by a number of anthropometric, kinematic and kinetic factors. These factors are subject-dependent and take effects at both musculoskeletal and organ level. Therefore, they cannot be properly considered by currently available single-level biomechanical models. Materials and Methods Based on our previous work [1, 2, 3], we developed a two-level biomechanical model to study how the mentioned factors affect hip fracture. The biomechanical model consists of a musculoskeletal dynamics model and a proximal-femur finite element model. Both of them were constructed from the patient's medical images and they are thus subject-specific. The dynamics model was applied to determine the impact force induced in sideways fall; the finite element model was used in computing the stress distributions in the proximal femur. Fracture risk index, defined using the actual and the ultimate stress, was used to measure hip fracture risk. Total 80 clinical cases were obtained from a local community clinical center of osteoporosis. For each case, the fracture risk was predicted by both a single- and the two-level biomechanical model. The effects of anthropometric parameters on hip fracture were investigated. Results and Conclusions The results revealed significant differences between the two types of models. Trends in the fracture risk predicted by the two-level model had much better agreement with the clinical observations reported in the literature. References [1] Y. Luo, Z. Ferdous and W.D. Leslie. A preliminary dual-energy X-ray absorptiometry-based finite element model for assessing osteoporotic hip fracture risk. Journal of Engineering in Medicine, Vol. 225, 1188 – 1195, 2011. [2] M. Nasirisarvi, Y. Luo, P. Sun and J. Ouyang. Experimental validation of subject-specific dynamic model for predicting impact force in sideways fall. Journal of Biomedical Science and Engineering, Vol. 7, 405 – 418, 2014. [3] Y. Luo, M. Nasirisarvi, P. Sun, W. Leslie and J. Ouyang. Prediction of impact force in sideways fall of the elderly by DXA-based subject-specific dynamics modelling. International Biomechanics, Vol. 1, 1 – 14, 2014.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Accuracy of Computation of Crystalline Defects at Fi nite Temperature

Author(s): Mitchell Luskin, ; Alexander Shapeev, *Skolkovo Inst. Sci. & Tech.*.

We present a theory of computation of crystalline defects at finite temperature. In a one-dimensional setting we introduce Gibbs distributions corresponding to such defects and rigorously establish their asymptotic expansion. We then give an example of using such asymptotic expansion to compare the accuracy of computations using free boundary conditions and using an atomistic-to-continuum coupling method. We will discuss extensions and applications of the theory to the computation of crystal defects at finite temperature for two and three dimensional problems.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Development of CSMM-Based Shell Element for Reinforced Concrete Structures

Author(s): Ken Luu, *U. Houston*.

The disastrous earthquakes caused heavy casualties and structural damage. It is found from the earthquake reconnaissance that shell-type reinforced concrete (RC) structures, such as nuclear containments, cooling towers, roof domes, shear walls, etc., are the key elements to resist earthquake disturbances. The shell-type RC structures can be visualized as assemblies of shell elements. The behavior of a whole structure can be predicted if the behavior of each shell element is thoroughly understood. This paper presents the development of a finite element analysis (FEA) program to predict the nonlinear behavior of RC shell structures. In the formulation, we utilize 8-node iso-parametric curved shell element and develop the constitutive relation modules with a multi-layer approach by taking into account the Cyclic Softened Membrane Model (CSMM) developed at the University of Houston. To form a FEA program, the constitutive relation modules and the analysis procedure were implemented into a finite element program development framework, OpenSees developed at UC Berkeley. Several large-scale structural tests were employed to validate the developed FEA program, including panels subjected to pure shear or combination of shear and bending, circular and rectangular hollow bridge columns and cylindrical tanks subjected to reversed cyclic loading.

13th U.S. National Congress on Computational Mechanics
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Title: Permeability in Multi-Porous Materials: A Multi-Scale Modeling Approach

Author(s): Hai Bang LY, Vincent Monchiet, *U. Paris-Est Marne la Vallée*; Daniel Grande, *U. Paris-Est Créteil*.

The elaboration and applications of porous materials have constituted areas of intense research for many years in the development of diverse applications, including materials for civil engineering, scaffolds for tissue engineering or devices for drug delivery applications. Over the last decade, doubly porous polymeric materials have attracted a particular attention from the research community. These particular materials offer new interesting perspectives for the preparation of sustainable materials. The role of each porosity level is different and associated with diverse transfer processes. Macropores would allow macro-molecules flow through the material, while a nanoporous network would be dedicated to the passage of smaller molecules, thus acting as a second transport mechanism, especially when macropores are totally clogged. To finely estimate the transport properties of such materials, the development of models and up-scaling methods has been considered. Indeed, the determination of the permeability of porous media is important in several practical problems related to mechanics and civil engineering. The modeling of flow through doubly porous materials raises a number of fundamental and practical questions such as the role of each porosity level on the macroscopic permeability, as well as the optimization of the microstructure to specific applications. The development of adapted numerical tools to simulate the fluid flow in multiporous materials then appears to be of key importance. In this context, we have developed a double upscaling approach to compute the permeability of doubly porous polymeric materials by employing numerical tools based on Finite Element Method (FEM) and Fast Fourier Transform (FFT). Due to the presence of separated scales, i.e. the nanopores, the macropores and the macroscopic scale, the effective permeability is determined by a consecutive double homogenization procedure. By a first scale transition at the lower scale, we compute a mesoscopic permeability by resolving the Stokes equations associated with the fluid flow through the nanopores of polymers. At the intermediate scale, the flow is described by the Stokes equations in the macropores and by the Darcy law for the permeable solid containing the nanopores, in order to finally compute the macroscopic permeability at the upper scale by a second scale transition. The latter is obtained by solving the coupled Stokes and Darcy problem. Finally, various illustrations are provided by considering different pore configurations for which the macropores are interconnected or not.

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Title: Dynamic Gouge Compaction and Dilatancy as a Simple Mechanism for Fault Zone Weakening and Short-Duration Slip Pulses

Author(s): Shuo Ma, Evan Hirakawa, *San Diego State U.*.

Triaxial experiments show that samples of fault gouge deform distinctly differently than those from the adjacent fault damage zone (e.g., Chester and Logan, 1986). Rock samples in the damage zone follow a characteristic elastic-brittle behavior, whereas fault gouge readily compacts and deforms in a more ductile manner. In order to explain the apparent weakness of large plate bounding faults such as the San Andreas Fault, Sleep and Blanpied (1992) proposed a mechanism in which compaction during interseismic creep reduces available pore space and hence increases fluid pressure. However, Segall and Rice (1995) questioned elevated pore pressure in the interseismic period in that it stabilizes the fault. Here we invoke a similar concept, however in this case the compaction process occurs dynamically via the stresses associated with earthquake rupture. We incorporate undrained compaction into a dynamic rupture model of a strike-slip fault with a strongly velocity-weakening friction (in a rate-and-state framework). A 20-cm thick fault gouge layer is modeled by an end-cap failure criterion (e.g. Wong et al., 1997) and experiences compaction and dilatancy, while the remainder of the model domain obeys the standard Mohr-Coulomb criterion. We show that large dynamic stresses associated with rupture propagation cause the gouge layer to compact ahead of the rupture front, leading to rapidly elevated pore pressure in the undrained fault zone and significant dynamic weakening of the principal fault surface. Compared to other dynamic weakening mechanisms such as flash heating and thermal pressurization, this mechanism does not require slip to initiate. Weakening ahead of the rupture front lowers the peak strength of the fault, leading to a lower strength drop on the fault. After the passing of the rupture front, strong dilatancy of undrained fault gouge reduces the pore pressure and restrengthens the fault, promoting a more pulse-like rupture.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Implementation of Complex Friction Laws in ABAQUS for Earthquake Dynamic Rupture Simulations

Author(s): Xiao Ma, *U. Illinois* ; Ahmed Elbanna, *U. Illinois*.

Computational modeling of earthquake ruptures represent a challenging class of initial-boundary value problem due to the vast range of spatial and temporal scales involved in the fracture process. An improperly chosen friction law may provide boundary conditions that render the elastodynamic problem ill-posed. Examples of these laws include Coulomb-Amonton friction and pure rate weakening laws. In this talk, we will present an implementation, in the Finite Element Software ABAQUS, of a more realistic description of friction that is consistent with well-controlled laboratory experiments. We will discuss two examples of these friction laws: slip-weakening and rate-and-state laws. Our objective is to leverage the finite element infrastructure provided by the software, which is accessible to a wide range of users, and complement it with a more realistic description of friction that is backed by experimental observations. We hope that this step will facilitate the usage of better friction models in applications that go beyond earthquake modeling such as in machine design and fiber reinforced composites. We discuss the challenges encountered in modifying the Vfric subroutine. We validate our implementation by comparing our model results with several problems in the Southern California Earthqauke Center Code Validation Exercise Archive.

13th U.S. National Congress on Computational Mechanics
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Title: Numerical Simulation of Shock Wave Interaction with a Deformable Particle Based on the Pseudo Arc-Length Method

Author(s): Xing Wang, Jianguo Ning, Tianbao Ma, *Beijing Inst. Tech.*.

The addition of metal particles to condensed phase explosives has become a common approach to change the total energy release of an explosive system. In this physical process, the early-time interaction of shock waves with the deformable particles is an important fundamental problem. The experimental and theoretical studies of shock interaction with deformable particles are extremely challenging because of its highly transient nature. As a result, no accurate mathematical model and numerical method exist yet that can be used in simulations. The objective of this paper is to combine the pseudo arc-length numerical method with the mathematical model of multiphase compressible flow for the simulation of shock wave interaction with a deformable particle. Firstly, an arc-length parameter is introduced to weaken the discontinuous singularity of hyperbolic partial differential equations, and then an efficient pseudo arc-length numerical method of multiphase compressible flow is proposed. Finally, the multiphase pseudo arc-length numerical method is applied to the problem of interaction between shock wave and the deformable particle. Through the flow flied changes and data analysis of key points, it can be found that the complex wave structures are presented after the interactions between the planar incident shock wave and the metal particle, and all these waves interaction will lead to the deformation of metal particle, then the deformable particle will affect the transmitted shock wave back. According to the discussion, the deformation of particle and shock wave propagation in the particle are determined by the shock wave impedance of each medium of explosive and shock speed, so the interaction between shock wave and the deformable particle can be studied on the basis of physical properties of explosive mediums. REFERENCES X. Wang, T.B Ma, J.G. Ning. A Pseudo Arc-Length Method for Numerical Simulation of Shock Waves. Chinese Physics Letter, 31(3), 030201, 2014. Y. Ling, A. Haselbacher, S. Balachandar, F. M. Najjar, D. S. Stewart. Shock interaction with a deformable particle: Direct numerical simulation and point-particle modeling. Journal of Applied Physics, 113(1), 013504, 2013. R. C. Ripley. Acceleration and heating of metal particles in condensed matter detonation. Ph.D. dissertation. University of Waterloo, 2010.

13th U.S. National Congress on Computational Mechanics
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Title: Damage Evolution of Fibre Metal Laminates Under Low Velocity Impact Loading: Experimental and Modeling

Author(s): Yu E Ma, Bo Wang, *Northwestern Polytech. U.*.

Fibre metal laminates(FMLs) is a type of hybrid material which consists of alternating layers of thin metallic sheets bonded together with fibre reinforced layers. With excellent mechanical properties, FMLs has become one of popular materials in aircraft structure application in recent years. Therefore, the low velocity impact tests of domestic FMLs and numerical analysis method were deeply studied in this paper. A range of low velocity impact tests with different energies were performed on domestic FMLs by Instron 9250 drop weight impact test machine. Visual damage on the surfaces and impact response of samples under different impact energies were analyzed. The effects of two boundary conditions with clamped and simply supported and the rolling direction of aluminium layers on the impact resistance of FMLs were studied respectively, and the low velocity impact responding mechanism of FMLs was analyzed as well. It shows that the boundary conditions have a certain effect on the impact response of FMLs, while the impact resistance of FMLs with different rolling direction of aluminium layers doesn't change greatly. The 3D composite damage model based on continuum damage mechanics was inferred and established and the relevant VUMAT was then programmed. A numerical analysis model of the low velocity impact of FMLs was established by the ABAQUS software, and it was then verified by experimental results. The impact damage of FMLs under typical test condition was mainly analyzed by numerical calculation, and the impact response characteristics at different stages were worked out. The damage type and response of each layer of FMLs during impact process were studied. And, the effect of size and shape of samples, thickness of aluminum layer and the number of metal/composite layers on the impact resistance of FMLs were investigated. Consequently, every sudden drop in the force-time curve exactly corresponds to an emergent failure in the FMLs. The more the delamination on both sides of aluminium layer, the less is the delamination between adjacent 90 degrees fibre layers. The results provide basic information and analysis method to design FMLs.

13th U.S. National Congress on Computational Mechanics
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Title: Numerical Verification of Local Eshelby Matrix in 2-D Eigen-Variable Boundary Integral Equations for Particles/Cracks in Full Space

Author(s): Hang Ma, *Shanghai U.*.

The eigen-variable boundary integral equation (BIE) method is proposed to reduce the solution scale and improve the efficiency encountered in the numerical simulation of solids with large number of particles/cracks. The definition of the eigen-variable consists of eigenstrain for particles and eigen COD for cracks [1-2]. With the eigen-variable BIE, the multiple particle/crack problems can be solved with the displacement discontinuity BIE in an iterative fashion with a small size of system matrix since the variables either on the interfaces of particle or on the surfaces of crack does not appear directly in the system equation. The local Eshelby matrix, i.e., the discrete form of the eigen-variable BIE in full space after group definition after dividing [3], is introduced into the BIE to deal with the interactions among particles/cracks, which is considered as a key step of the method to guarantee the convergence of iteration. In the present work, numerical verifications of local Eshelby matrix in 2-D eigen-variable BIE are carried out taking a small number of particles/cracks in full space, compared with the results of the dual BIE method with domain decomposition, showing the effectiveness and the efficiency of the proposed method. Keywords: eigenstrain, eigen COD, local Eshelby matrix, boundary integral equation, particles, cracks

_____ *E-mail address: hangma@staff.shu.edu.cn (H.Ma) Acknowledgement: The work was supported by the National Natural Science Foundation of China (No.11272195).

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13th U.S. National Congress on Computational Mechanics
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Title: Design of Experiments for Uncertainty Quantification of FEA Modeling in DMLS Additive Manufacturing

Author(s): Li Ma, Jeffrey Fong, Brandon Lane, Shawn Moylan, Lyle Levine, *NIST*.

Direct metal laser sintering (DMLS) is an additive manufacturing (AM) technology for the fabrication of near net shaped parts directly from computer-aided design (CAD) data by melting layers of metal powder with a laser source. DMLS is one of the most promising additive manufacturing processes with better surface and geometric part qualities compared to other metal AM technologies. However, the highly localized laser power input leads to extremely high local temperature gradients. As a result, significant residual stress, distortion, and defects to the workpiece may occur. DMLS finite element analysis (FEA) modeling plays an important role in understanding the process, predicting optimal fabrication strategies, and qualifying fabricated parts based on those strategies. However, there remain significant challenges to constructing accurate FE simulations of the DMLS process. In this research, 3D thermal finite element analysis (FEA) models of DMLS were developed. The FEA DMLS thermal models incorporate a continuous moving heat source, phase changes, and powder thermal property changes after melting, etc. Several laser scans on both one layer of metal powder and on solid metal substrates were modeled. Meanwhile, the same scans were processed on NIST's EOS M270 DMLS machine. Temperature results from in-situ thermographic measurements were compared with that of the FEA modeling and showed agreement. In the AM simulation, input of accurate material and simulation parameters is critical for accurate prediction of process signatures. It is challenging and expensive to measure and control all possible material properties and process parameters. In this research, we applied a design of experiment approach which varied simulation parameters to evaluate the uncertainty quantification of DMLS FEA modeling results. Design of experiments provides an exploratory tool to weigh large number of factors, optimize alternative modeling approaches, and determine which of the many approaches can predict AM process performance for quality control.

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Title: Accelerated Model-Based Signal Reconstruction for Magnetic Resonance Thermometry Data in Presence of Uncertainties

Author(s): Reza Madankan, David Fuentes, *MD Anderson Cancer Center*.

An accelerated model-based information theoretic approach is developed to perform the task of image reconstruction from observed k-space samples in Magnetic Resonance Imaging (MRI). The key idea of the proposed approach is to optimally detect k-space regions of high information content with respect to sensor models of MR thermometry. A combination of uncertainty quantification and information theoretic techniques are used to locate k-space regions that demonstrate the highest sensitivity with respect to a composite heat transfer and MR physics. The key contribution of this method is to optimally select the samples on k-space such that they result in efficient estimates of the corresponding temperature map. Optimally selected observations on k-space are utilized to refine the model and the refined model is then used to generate the temperature field corresponding to the observations. Performance of proposed approach is demonstrated in-silico as well as retrospectively in-vivo human data.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Peridynamics for Modeling Crack Formation and Growth in Nuclear Fuel Pellets

Author(s): Erdogan Madenci, Selda Oterkus, *U. Arizona*.

The degraded physical state of fuel becomes the limiting factor with regard to long term and transient reactor performance. Specifically, as the fission inducing neutrons interact with fuel nuclei, the fuel experiences loss of structural integrity. Changes in the mechanical and thermal properties of fuel, because of burnup, have a major impact on performance. As the fuel heats up, cracking occurs radially inward toward the fuel center. During steady-state operation, annealing occurs centrally leaving a circumferential crack pattern. The various cracking patterns during operation significantly affect the fuel thermal conductivity and neutron diffusion coefficient and therefore feed back into the overall pellet thermal- expansion influencing gap closure. Thus, the analysis of fuel pellet behavior is truly representative of a thermal, mechanical and neutronic multiphysical interaction. Currently, a truly predictive all-inclusive analysis and simulation tool that couples heat diffusion with mechanical material interaction in conjunction with realistic fracture mechanics does not exist. This study presents the capability of peridynamics for addressing multiphysics problems, specifically fuel pellet cracking prediction without the effect of neutronics. The fully coupled field equations of heat and oxygen diffusion and deformation are solved in one framework. Cracking in each field is reflected immediately by using the same computational discretization for each field equation. Also, the time dependent material behavior as well as their variability are included in the analysis.

13th U.S. National Congress on Computational Mechanics
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Title: A Bayesian Approach to Selecting Hyperelastic Constitutive Models of Soft Tissue

Author(s): Sandeep Madireddy, Kumar Vemaganti, *U. Cincinnati*; Bhargava Sista, *ANSYS*.

Hyperelastic constitutive models of soft tissue mechanical behavior are widely used in applications ranging from traumatic brain injury simulation to computer-aided surgery and functional tissue engineering. While numerous constitutive models have been proposed in the literature, an objective method is needed to select a parsimonious model that represents the experimental data well and has good predictive capability. This is an important problem given the large variability in the data inherent to soft tissue mechanical testing. In this talk, we discuss a Bayesian approach to this problem based on Bayes factors. We propose a holistic framework for model selection, wherein four different factors are used to reliably choose a parsimonious model from the candidate set of models. These are the qualitative fit of the model to the experimental data, evidence values, maximum likelihood values, and the landscape of the likelihood function. We consider three hyperelastic constitutive models that are widely used in soft tissue mechanics: Mooney-Rivlin, Ogden and exponential. The mechanical testing data from the literature for bovine liver tissue is used to calculate the model selection statistics. A nested sampling approach is used to evaluate the evidence integrals and other statistics in the Bayesian approach. In our results, we highlight the robustness of the proposed Bayesian approach to model selection compared to the likelihood ratio, and discuss the use of the four factors to draw a complete picture of the model selection problem, which is used to rank the models in the order of their usability.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling of Polymer Blends with Diffuse Interfaces and Free Surface Through the Cahn-Hilliard Equation

Author(s): Santiago Madruga, *U. Politécnica-Madrid*; Fathi Bribesh, *Zawia U.*; Uwe Thiele, *U. Münster* .

Stable, unstable and metastable structuring of confined polymer blends at off-critical concentrations deposited on a solid substrate and with a free evolving surface is presented. The non-linear solutions are obtained numerically using a variational form of the Cahn-Hilliard equation in the static limit, which allows for internal diffuse interfaces between the two components of the mixture. The upper free surface is sharp and free to move, allowing strong deformations. Varying the average composition, the size of the films and the surface energy we find a rich morphology of static films in the form of laterally structure films, layered films, droplets on the substrate, droplets on the free surface, and checkerboard structures. We show that structured solutions are energetically favorable over homogeneous states within the whole spinodal region and find the states of absolute stability. Existence of most of the branches of non-linear solutions at off-critical mixture concentrations can be predicted from the knowledge of the non-linear solutions at critical compositions plus the branching points at off-critical compositions derived from a simple linear stability analysis. However, some families of solutions have no correspondence at critical compositions [1]. We study as well the transport by convection through the named model-H, which generalizes the Cahn-Hilliard model by coupling the momentum transport to diffusion of the components. Model-H is extended to account for free surface boundary conditions allowing us to study the combined effect of phase separation within a film of polymer blend and structuring of the surface of the film itself [2]. We apply it to analyze the stability of vertically stratified steady extended films and show that convective transport leads to new mechanisms of instability as compared to the simpler purely diffusive case described by the Cahn-Hilliard model [3]. Santiago Madruga acknowledges support by the Spanish Ministerio de Economa y Competitividad via the projects TRA2013-45808-R and ESP2013-45432-P. [1] F. Bribesh, S. Madruga and U. Thiele. Two-dimensional steady states in off-critical mixtures with high interface tension. Eur. Phys. J. Spec. Top. 219:3-12, 2013. [2] U. Thiele, S. Madruga, and L. Frastia. Decomposition driven interface evolution for layers of binary mixtures: I. model derivation and base states. Phys. Fluids, 19:122106, 2007. [3] S. Madruga and U. Thiele. Decomposition driven interface evolution for layers of binary mixtures: II. influence of convective transport on linear stability. Phys. Fluids, 21:062104, 2009.

13th U.S. National Congress on Computational Mechanics
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Title: Compression-Loose Fiber Media: Continuum Constitutive Law and Single Crack Case-Study

Author(s): Omar Mahmood, *UPMC U. Paris* ; Basile Audoly, *UPMC U. Paris*; David Rodney, *U. Lyon*; Stephane Roux, *U. Paris-Saclay*.

A particular aspect of fiber network materials is that they exhibit a different stiffness in traction and in compression [1]. This nonlinearity is mainly due to the local buckling of fibers. We analyze the global response of a fiber network comprising a pre-existing crack: in this geometry the strain is inhomogeneous and the material nonlinearity dramatically affects the distribution of stress. We first derive a continuum model representing a 2D network of springs (fibers) whose stiffness in compression is a fraction of the stiffness in extension. Within the framework of a directional constitutive model, a continuous elastic energy density is obtained from integrating the fiber extensions over all spatial directions. This elastic energy is quadratic homogeneous with respect to the isotropic strain intensity, but exhibit a particular behavior with an anisotropic strain. The equivalent continuum is Hookean when fibers have identical modulus in traction and compression, but nonlinear for bi-modulus fibers. We are particularly interested in the asymptotical case of fibers with zero stiffness in compression (unilateral constitutive law), corresponding to an elastic medium which is soft in compression. The homogenized constitutive law is implemented in a finite element model (FEM) where the derivatives of energy density are evaluated through an automatic differentiation method (see [3] for details). We study the influence of the fiber nonlinearity, and compare simulations of a discrete network of springs to FEM simulations based on the continuous equivalent medium. The stress around the crack tip is analyzed and compared with the classical asymptotic from linear elastic fracture mechanics. We also explain the emergence of unloaded area (both principal strains are compressive) on both sides of the crack. Then, we highlight the strain-induced anisotropy (orientation of buckled fibers) around the crack. The propagation of this anisotropy when increasing the fiber nonlinearity is discussed. In particular, we find that a diamond shaped area is progressively unloaded as the fiber nonlinearity increases. References: [1] L. Mezeix, C. Bouvet, J. Huez, D. Poquillon, Journal of Material Sciences, 44:3652-3661 (2009) [2] J. A. Åström, J. P. Mäkinen, M. J. Alava, J. Timonen, Phys. Rev. E, 61:5550-5556 (2000) [3] C. Bendtsen, O. Stauning, Technical Report: IMM-REP-1996-17, Technical University of Denmark (1996)

13th U.S. National Congress on Computational Mechanics
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Title: Pick Your Pole: Modeling the Subcellular Processes of Polarity Selection Cycles in Myxobacteria

Author(s): Shant Mahserejian, Francesco Pancaldi, Jianxu Chen, Chinedu Madukoma, Danny Chen, Joshua Shrout, Mark Alber, *U. Notre Dame*.

The characteristic motility features of the rod shaped myxobacteria make them a model organism for studying polarity selection. A mathematical model is presented to describe distributions of the RomR protein at the poles inside the cell body, the fluctuations of which lead to changing polarity and thus direction of motion. This work involved tracking the RomR protein during in vivo experiments with gfp-labeled M. xanthus using high temporal resolution fluorescent microscopy, and high frequency analysis was used to reach our findings. We tested previous results on the asymmetric distributions of RomR during polarity selection, as well as establish the possible mechanisms involved in RomR transport leading to the reset of polarity during cell reversal and division events.

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Title: An Agglomerated Multi-Grid Algorithm for Steady Compressible Flows with Embedded Boundaries

Author(s): Alex Main, *Duke U.*.

This talk examines the construction of agglomerated multigrid methods for problems involving steady, compressible flow with embedded boundaries. The utility of multigrid methods to accelerate the convergence of steady fluid flow computations, especially for those at low mach numbers, has been well attested to in the literature. Good results have also been demonstrated for purely hyperbolic equations (e.g., the Euler equations) as well as for the full Navier-Stokes equations. In particular, for unstructured grids with body-fitted boundaries, agglomerated multigrid methods have been shown to be efficacious [1]. We combine the agglomerated multigrid technique with the FIVER [2] technique for discretizing the compressible (viscous or inviscid) flow equations on unstructured grids with embedded boundaries. In particular, two challenges are addressed within this context: first, how to construct the agglomerated coarse meshes and coarse grid equations with FIVER and second, how to transfer the solutions between grids. Computational results will be presented for both the Euler equations and the compressible Navier-Stokes equations. The computational performance is assessed by comparing the overall simulation time required by the embedded multigrid scheme against both a single grid scheme and a state of the art Newton-Krylov solver [3]. Specifically, the multigrid scheme for steady flows provides for realistic problems speedups of between 1.5 and 8x over a Newton-Krylov method. Finally, directions for future research will be discussed. [1] Mavriplis D. Directional agglomeration multigrid techniques for high-reynolds- number viscous flows. AIAA journal, 37(10):1222–1230, 1999. [2] Farhat C., Gerbeau J-F., and Rallu A. Fiver: A finite volume method based on exact two-phase riemann problems and sparse grids for multi-material flows with large density jumps. Journal of Computational Physics, 231(19):6360– 6379, 2012. [3] Main A. and Farhat C. A second-order time-accurate implicit finite volume method with exact two-phase riemann problems for compressible multi-phase fluid and fluid–structure problems. Journal of Computational Physics, 258:613– 633, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: Mixed Hybrid Finite-Element Modeling of Hydrated Porous Media (Finite Deformation)

Author(s): K Malakpoor, J.M Huyghe, C Yu, *Eindhoven U. Tech.*.

Biological, mineral, and synthetic porous media exhibit swelling when in contact with changing salt concentrations. This swelling is caused by two factors: Donnan osmotic swelling and hydration or adsorption forces. Donnan osmosis is associated with electrical charges fixed to the solid, counteracted by corresponding charges in the fluid, which in turn attracts water, whereas, hydration results from the ordering of polar water molecules. As a consequence of the fixed charges a variety of physical phenomena are observed in these materials, such as streaming potentials, diffusion potentials, electro-osmosis, electro-phoresis. Swelling porous materials have numerous applications in industry: sealing of leakage, adsorption of waste liquids in the field of personal hygiene, reservoir engineering, etc. Porous materials that are used for industrial applications, such as personal hygiene articles, clays and intervertebral discs must perform under a wide range of usage conditions. Osmoelastic media have large negatively charged groups attached to the solid matrix. Due to the fixed charges, the total ion concentration inside the medium is higher than in the surrounding fluid. This excess of ion particles leads to an osmotic pressure difference, which causes swelling of the medium. The resulting equation describing the mentioned phenomena is strongly non-linear coupled equations of the deformation and convection-diffusion of fluid and solutes. It is shown that mixed hybrid formulation yields much more accurate results for this highly coupled problem. thanks to its local mass conservation. In this paper it is shown that mixed hybrid finite element has major advantages over conforming elements in highly coupled multicomponent analyses even when no discontinuities are involved. Because of the interplay of the strong non- linearities of the system with convection-diffusion of the ions, filtration and osmosis of the water and 3D finite deformation of the macromolecular network, violations of local mass balance may result in lack of the stability of the Newton-Raphson iterative convergence procedure.

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Title: Multi-Scale Modeling of Deformation Behavior in Near Beta Ti-5553 Alloy

Author(s): Sudipto Mandal, Anthony Rollett, *Carnegie Mellon U.*; Shanoob Balachandran, Dipankar Banerjee, *Indian Inst. Sci. Bangalore*.

Titanium alloy 5553 is a near beta alloy, which is recently being used in aircraft components due to their excellent mechanical properties. A viscoplastic self-consistent code (VPSC) is used to determine hardening parameters in order to match the experimental stress-strain behavior at different temperatures and strain rates [1]. Synthetic 3D microstructures are created to mimic the crystallographic features, grain size and grain shape distribution of measured microstructures of the Ti-5553 alloy. The deformation behavior of the synthetic microstructures is studied by observing changes in microstructure and texture using viscoplastic FFT codes using the optimized parameters. The elasto-viscoplastic response of the synthetic microstructures with different morphologies and fractions of alpha phase particles are also examined using an elasto-viscoplastic FFT code [2]. The alpha morphology is found to have a significant effect on the mechanical response. This then permits a rationalization of the softening behavior observed in stress-strain tests at high temperatures. Both the macroscopic and microscopic responses of the synthetic microstructures are compared with data from experiment and literature. This work is supported by the Boeing company. [1] R.A. Lebensohn and C. N. Tomé. "A self-consistent viscoplastic model: prediction of rolling textures of anisotropic polycrystals." Materials Science and Engineering: A 175.1 (1994): 71-82. [2] R.A. Lebensohn, A.K. Kanjarla and P. Eisenlohr. "An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials." International Journal of Plasticity 32 (2012): 59-69.

13th U.S. National Congress on Computational Mechanics
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Title: The Buckling Sphere: A Symbiosis of Mechanics and Geometry

Author(s): Herbert A. Mang, Xin Jia, Stefan Pavlicek, *Vienna U. Tech.*.

The task of this presentation about work in progress is to prove theoretically and numerically that a specific linear eigenproblem in the framework of the Finite Element Method (FEM), referred to as the consistently linearized eigenproblem (CLE), has amazing physical properties. They can be exploited for computation of the ratio of the membrane strain energy over the total strain energy in the entire prebuckling regime and at the stability limit, which may either be a bifurcation point or a snap-through point. Normalization of that one eigenvector which is part of the fundamental eigenpair such that its length is equal to one results in a surface curve on a unit (hemi)sphere. For convenience, it is referred to as the buckling sphere. The fundamental eigenpair is defined as that one, whose eigenvalue becomes zero at the stability limit. It is a function of a dimensionless load parameter which is increased up to the stability limit. The symbiosis of mechanics and geometry is reflected by the zenith angle and the azimuth angle, representing the two spherical coordinates that define the position of an arbitrary point on the surface curve described by the vertex of the fundamental eigenvector of the CLE. The spherical coordinates depend on this eigenvector, which in turn depends on the load parameter. The underlying hypothesis is that the radius of curvature at an arbitrary point of the surface curve is equal to the aforementioned energy ratio. So far, this hypothesis was verified numerically for the two energetical limiting cases, i.e. for a membrane stress state and a pure bending stress state. Based on this hypothesis, the radius of curvature of the surface curve can be set equal to the square of the sine of the zenith angle. This implies that the pole of the equator correlates with a pure bending stress state. Once the zenith angle is known, the azimuth angle can be determined. It is a measure of the degree of nonlinearity of the underlying structural problem in the prebuckling regime. The presentation consists of the formulation of the hypothesis, the proof that the CLE is indeed the tool needed for accomplishing the task of this work, and the numerical investigation of the two limiting cases including comments on the algorithmic translation of the theory. Depending on further progress of their research, the authors also intend to report on the numerical verification of the general case.

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Title: Calibration and Validation of A Sand Plasticity Model for Liquefaction Analysis

Author(s): Majid Manzari, *George Washington U.*.

Majority of the advanced numerical procedures that are currently available for liquefaction analysis of geo-structural systems are based on an effective stress formulation in which displacement of soil skeleton and pore water pressure (and possibly the pore fluid displacements) serve as the primary unknowns. To be suitable for liquefaction analysis, these procedures must use a constitutive model that can accurately simulate the salient features of the stress-strain response of soil skeleton over a wide range of strains, soil densities, and effective stresses. Appropriate modeling of the pore fluid motion and it potential migration is also a critical factor affecting the liquefaction-induced deformations of geo-structural systems during and after the shaking phase. In this work, a critical state soil plasticity model for sands is first calibrated by using an extensive set of monotonic and cyclic shear tests. The calibrated model is then used in a series of fully-coupled effective stress finite element analyses to simulate the seismic response of the selected sandy soil in increasingly complex configurations. It is shown that while calibration of the constitutive model using the element tests is crucial step for a successful simulation, a few other elements of the analytical/numerical analysis procedure such as constitutive response of the pore fluid, small strain stiffness degradation and damping characteristics of the soil also play important roles.

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Title: Virtual Elements and Mimetic Methods

Author(s): Gianmarco Manzini, *Los Alamos Nat'l. Lab.*.

We present a family of schemes for solving elliptic partial differential equations on unstructured polygonal and polyhedral meshes. These discretizations can be interpreted in the framework of mimetic finite difference methods and virtual element methods. As mimetic methods, they are built to satisfy local consistency and stability conditions. The consistency condition, which ensures the well-posedness of the method, is an exactness property, i.e., all the schemes of the family are exact when the solution is a polynomial of an assigned degree. The degrees of freedom are the solution moments on mesh faces and inside mesh cells, thus resulting in a non-conforming discretization. Higher order schemes are built using higher order moments. The developed schemes are verified numerically on convection-diffusion-reaction problems with constant and spatially variable (possibly, discontinuous) tensorial coefficients.

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Title: Quasicontinuum Study of Three-Dimensional Crack Initiation Mechanisms in Bcc-Fe Under Loading Modes I, II and III

Author(s): Jaime Marian, *UCLA*.

We present quasicontinuum simulations of three-dimensional edge cracks in single crystal bcc-Fe. Crystals with different thicknesses and crystallographic orientations have been investigated and loaded in modes I, II and III. We study incipient plasticity at the crack tip and the onset of crack propagation, and calculate the critical stress intensity factors for crack propagation and dislocation emission. The active slip systems and the character of attendant dislocations have been identified and compared with the standard 2D behavior. We find that the observed type of propagation depends on the loading mode and crystallographic orientation. Mechanisms comprise twinning, bcc-fcc phase transformation, void formation and dislocation emission.

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Title: Hadamard Instability Analysis for Coupled Chemo-Thermo-Mechanical Systems

Author(s): Xanthippi Markenscoff, *UCSD*.

A Hadamard instabiblity analysis of the system of partial differential equations governing a coupled nonlinear chemo-thermo-mechanical system provides a unified analysis of both “spinodal” Larche-Cahn type (loss of convexity of thermodynamic functions) instabilities, and “negative creep” ones [1], by balancing different order terms in the eigenvalue equation[2,3]. [1] Li, J.C.M., “Negative creep and mechanochemical spinodal in amorphous metals” Materials Science and Engineering, 98, pp 465-468, 1988 [2]Markenscoff, X., “Instabilities of a thermo-mechano-chemical system”, Quart. Appl. Math., 59, pp 471-477 (2001) [3] Markenscoff, X. Hadamard instability analysis of “negative creep” in coupled chemo-thermo-mechanical systems, Continuum Mechanics and Thermodynamics, submitted

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Title: Stochastic Vortex Structure Method for Simulation of Interacting Particles in Turbulent Flows

Author(s): Jeffrey Marshall, Kyle Sala, Farzad Faraji Dizaji, *U. Vermont*.

Heavy particles are thrown out of turbulent eddies by centrifugal force, forming high concentration sheets lying between the eddy structures. The concentration heterogeneity caused by this dispersion process can have a significant impact on processes that depend on local particle concentration, such as particle collision rate and adhesion, triboelectrification, microorganism interactions, particle combustion, and chemical reactions between particles and the surrounding fluid. Since in most practical problems it is not possible to directly compute all scales of the turbulent flow, we must introduce a model for the scales of turbulence that are responsible for particle dispersion which is consistent with known averaged turbulence quantities. This works presents a discussion, evaluation and comparison of different stochastic methods for modeling the evolution of interacting particles in turbulent flows. The key flow quantities that are necessary to accurately predict dispersion and interaction in turbulent flows are identified and related to structural aspects of the flow. The accuracy of prediction of these flow features by different stochastic models are evaluated by comparison to direct numerical simulation. The stochastic Lagrangian method traditionally used for non-interacting particles, which involves solution of a stochastically-forced differential equation (e.g., the Langevin equation), is found to be highly inaccurate for modeling interacting particles. A new stochastic vortex structure (SVS) method is proposed which provides structural cohesiveness that is missing in stochastic Lagrangian methods. A fast SVS method is described based on a variation of the fast multipole approach, which together with parallelization enables speed-up of the simulations by several orders of magnitude. The properties of the synthetic turbulent flow generated by the SVS approach are examined, both in order to determine sensitivity of the SVS flow to different parameter values and to assess accuracy of the SVS predictions in comparison to turbulence DNS results. Use of SVS for prediction of particle collision rate in turbulent flows are then assessed in comparison to turbulence DNS.

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Title: Modelling the Fracture Processes of FRP-to-Concrete Interfaces Under Cyclic Actions

Author(s): Enzo Martinelli, *U. Salerno*; Antonio Caggiano, *CONICET & LMNI-UBA*.

The use of Fyber-Reinforced Polymers (FRPs) is getting more and more common in structural strengthening of existing constructions, as a result of their advantages in terms of efficiency and installation time. Although a big deal of research focused on the bond behaviour under monotonic actions, only few contributions are currently available for describing the response of FRP-to-concrete substrates under cyclic actions and, furthermore, they are generally limited to the quasi-static case. This work is intended at formulating a theoretical model capable of simulating the response of FRP strips glued to concrete and subjected to cyclic actions induced by dynamic load cases, such as the ones resulting in the anchorage zones of FRP strips employed in seismic retrofitting of concrete members. Although mixed fracture modes are often observed in debonding phenomena occurring at the FRP-to-concrete interface, the assumption of pure mode II is considered in this model, as often accepted within the scientific literature (Martinelli et al, 2011). The model is based on an incremental formulation inspired to the fundamental principles of both the flow theory of plasticity and fracture mechanics. Particularly, an exponential bond-slip law is assumed for simulating the monotonic behaviour of the FRP-to-concrete interface and damage is considered for simulating the local loading-unloading behaviour. Moreover, the strain-rate effect deriving by the dynamic nature of the applied cyclic actions is considered: a rate-dependent formulation developed according to the viscoplasticity theory is proposed with the aim of simulating the aforementioned dynamic effects. A finite difference solution (central in space, forward/backward in time) is proposed for implementing the aforementioned theoretical model in a numerical code capable of simulating the response of the structural systems under consideration under relevant cyclic actions (Martinelli & Caggiano, 2014). Finally, the thermodinamical consistency of the formulated model is discussed (Ragueneau et al, 2006) and the conditions under which it is actually met are clearly highlighted. References: Martinelli E., Caggiano A. (2014), A unified theoretical model for the monotonic and cyclic response of FRP strips glued to concrete, Polymers 6 (2), 370-381; Martinelli E., Czaderski C., Motavalli M. (2011), Modeling in-plane and out-of-plane displacement fields in pull-off tests on FRP strips, Engineering Structures 33 (12), 3715-3725 Ragueneau F., Dominguez N., Ibrahimbegovic A. (2006), Thermodynamic-based interface model for cohesive brittle materials: Application to bond slip in RC structures, Computer Methods in Applied Mechanics and Engineering, 195(52), 7249 – 7263.

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Title: Numerical Dispersion in Peridynamics: Quality Assessment and Comparative Study Including Finite Difference and Finite Element Methods for Analyses of Wave Propagation in Solids

Author(s): Adam Martowicz, Wieslaw J. Staszewski, Tadeusz Uhl, *AGH U. Sci. & Tech.*; Massimo Ruzzene, *Georgia Inst. Tech.*.

Peridynamics is a relatively new approach in the field of computational mechanics, originally proposed for modeling solids. It offers a wide range of valuable applications due to an integral-based mathematical problem description. First, different types of physical nonlinearities, especially including geometric discontinuities, can be easily considered in the model, since no gradient is required. Second, considered nonlocality opens new perspectives for more physical modeling of material properties, also for correct simulations of elastic waves propagation. Up to now, majority of the researchers' effort regarding peridynamics was put towards correct modeling of failure and its growth, also for complex media. Although there are known applications of peridynamics to analyses of wave propagation, damage induced changes in the wave properties, including acoustic emission, crack-wave interactions as well as wave modulations, there is still observed lack of comprehensive study on numerical aspects of peridynamic models, taking into account numerical dispersion and potential effects on its ignorance. The presented work is particularly devoted to the quality assessment for peridynamics in terms of mitigation of numerical dispersion as well as capabilities of correct recreation of physical dispersion. Peridynamics, through its nonlocal formulation for solid elasticity, thankfully features a perspective of effective influence of numerical dispersion. It appears when the time step or the lengthscale defined for a numerical model are improperly determined with respect to the frequencies and wavenumbers of the waves propagating in the model. Moreover, numerical dispersion is responsible for unwanted behavior in models with sharp interfaces and geometric discontinuities. Preventing from numerical dispersion in simulations should be considered as a critical issue. When being uncontrolled, numerical dispersion may lead to artifacts, non-physical dispersions and false wave scattering effects. The influence of this phenomenon may be, however, objectively assessed with either dispersion curves or the results of numerical analyses carried out to simulate the phenomenon of wave propagation, which is the case of the current work. Finally, the results of comparative study are presented to show the differences between the properties of peridynamics, FE and FD methods in terms of numerical dispersion. The work was supported by the Foundation for Polish Science (FNP-WELCOME/2010-3/2). References W. Hu, Y.D. Ha, F. Bobaru 2012 Computer Methods in Applied Mechanics and Engineering. 217–220, 247–261. A. Martowicz, W.J. Staszewski, M. Ruzzene, and T. Uhl 2014 Vibro-acoustic wave interaction in cracked plate modeled with peridynamics. Proceedings of the WCCM XI-ECCM V-ECFD VI, Barcelona, Spain, 20-25 July 2014.

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Title: A Cut Discontinuous Galerkin Method for the Laplace-Beltrami Operator with Applications to Surface-Bulk Problems

Author(s): Erik Burman, *U. College London*; Peter Hansbo, *Jönköping U.*; Mats G. Larson, Andre Massing, *Umeå U.*.

In this talk, we consider a discontinuous Galerkin method for the Laplace-Beltrami prob- lem on a smooth two dimensional surface embedded into a three dimensional space meshed with tetrahedra. Since the surface is not aligned with mesh, we use the trace of discontin- uous piecewise linears defined on the tetrahedra as trial and test functions in the discrete variational formulation. As the resulting linear system may be severely ill-conditioned due to possibly small intersections between the surface and the mesh, consistent stabiliza- tions terms are added to the original bilinear form. The proposed discretization scheme has optimal convergence properties and give raise to a well-conditioned discrete linear system independent of the intersection configuration. We conclude the presentation by il- lustrating the theoretical findings by a series of numerical experiments. As an application example, we consider the flow in porous media with fractures/faults, demonstrating the capability of our methods to compute the Darcy flow for a coupled surface-bulk problem when flow is present in both the crack surface and the bulk of the porous medium.

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Title: A Heterogeneous Modeling Method with Embedded Interfaces for Porous Media Flows

Author(s): Arif Masud, Georgette Hlepas, *U. Illinois, Urbana-Champaign*; Timothy Truster, *U. Tennessee*.

This talk presents a new heterogeneous multiscale modeling method for porous media flows. Physics at the global level is governed by one set of partial differential equations, while features in the solution that are beyond the resolution capacity of the global model are accounted for by the next refined set of governing equations (1,2). In this method, the global or coarse model is given by the Darcy equation while the local or refined model is given by the Darcy-Stokes equation. Concurrent domain decomposition where global and local models are applied to adjacent sub-domains, as well as overlapping domain decomposition where global and local models co-exist on overlapping domains, is considered. An interface operator is developed for the case where global and local models commute along the common interface. We adopt the procedure proposed in (3) to derive a primal interface operator with the character of a Discontinuous Galerkin (DG) method by starting from a Lagrange multiplier interface formulation. This approach relies crucially on applying concepts from the VMS method locally at the interface between the local and global models to derive the numerical flux terms for the DG method (4), which allows for different element types and jumps in material properties between the two models. For the overlapping decomposition a residual based coupling technique is developed that consistently facilitates bottom-up embedding of scale effects from the local Darcy-Stokes model into the global Darcy model. Numerical results are presented for non-overlapping as well as overlapping domain decompositions for various benchmark problems. References: (1) A. Masud and G. Scovazzi, A heterogeneous multiscale modeling framework for hierarchical systems of partial differential equations. International Journal for Numerical Methods in Fluids, vol. 65, 28-42, 2011. (2) G. Hlepas and A. Masud, A Heterogeneous Model for Porous Media Flows,■ International Journal for Numerical Methods in Fluids, Vol. 75:487–518, 2014. (3) T.J. Truster and A. Masud, Primal interface formulation for coupling multiple PDEs: A consistent derivation via the Variational Multiscale method. Computer Methods in Applied Mechanics and Engineering, vol. 268, 194-224, 2014. (4) T.J.R. Hughes, A. Masud and J. Wan, “A Discontinuous-Galerkin Finite Element Method for Darcy Flow,” Computer Methods in Applied Mech and Engrg, 195, pp. 2102-2137, 2005.

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Title: On Locking-Free Methods for Isogeometric Large Deformation Analysis of Geometrically Exact Three-Dimensional Beams

Author(s): Kjell Magne Mathisen, Tore Andreas Helgedagsrud, Siv Bente Raknes, Bjørn Haugen, *Norwegian U. Sci. & Tech.*; Knut Morten Okstad, *SINTEF* ; Trond Kvamsdal, *SINTEF* .

In this work the geometrically exact three-dimensional (3D) beam theory of Reissner [1], and later revisited by Simo [2], has been used as basis for development of a variety of isogeometric large deformation 3D beam elements. Geometrically exact 3D beam theory has no restrictions with respect to size of displacements, rotations and deformations. Ibrahimbegovic [3] has shown that an improved representation of the curved reference geometry significantly increases the accuracy of the results. Whereas earlier studies [3] utilized C0-continuous Lagrange polynomials, we use NURBS shape functions, for approximation of both geometry and displacements. While reduced integration may be used to alleviate transverse shear and membrane locking in standard C0-continuous Lagrange elements this does not automatically extend to isogeometric elements. In this study we investigate how optimal patch-wise numerical quadrature rules and linked interpolation may be used to obtain locking-free isogeometric large deformation geometrically exact 3D beams. A range of numerical examples serves to illustrate and assess the performance compared to traditional Lagrange interpolated elements. [1] E. Reissner, “On finite deformations of space curved beams”, J. Appl. Math. Phys., 32, 734–744, (1981). [2] J.C. Simo, “A finite strain beam formulation”, Comput. Meth. Appl. Mech. Engrg., 49, 55–70, (1985). [3] A. Ibrahimbegovic, “Finite element implementation of Reissner’s geometrically nonlinear beam theory: three-dimensional curved beam finite elements”, Comput. Meth. Appl. Mech. Engrg., 122, 10–26, (1995).

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Title: Image--Based, High-Performance Multi-Scale Modeling

Author(s): Karel Matous, Matthew Mosby, *U. Notre Dame*.

With concentrated efforts from the material science community to develop new multi-functional materials, that inherently span several length scales, the need for modeling tools that accurately describe the physical phenomena at each scale has only further been emphasized. Therefore, we will present a multiscale framework, for modeling the macroscopic/mesoscopic behavior of heterogeneous materials and heterogeneous material layers in particular, capable of capturing the large range of spatial scales. The multiscale cohesive model is based on the Hill's Lemma and couples physical processes at the mesoscale to the macroscopic response in order to derive a homogenized cohesive law. Simulations involving this wide range of scales are inherently expensive, requiring the use of high-performance computing. Therefore, we develop a hierarchically parallel high-performance computational framework that executes on tens of thousands of processing cores. Any serious attempt to model a heterogeneous system must also include a strategy for constructing a complex computational domain. This work follows the concept of data-driven (image-based) modeling. We will delineate a procedure based on topology optimization to construct a Representative Unit Cell (RUC) with the same statistics (n-point probability functions) to that of the original material. Our current micro-computed-tomography (micro-CT) instrument provides tomographic imaging of a material structure with ~3 μm resolution, resulting in a direct link between experimental observations and the material system. We show that high-performance direct numerical simulations of these statistically meaningful mesoscopic domains are possible. Therefore, well-resolved mesostructure-statistics- property relationships can be obtained. Moreover, fully coupled multiscale simulations of complex nonlinear processes will be presented. Finally, micro-CT can become a much more powerful tool by combining it with quantitative abilities for complete comparison with the corresponding simulations. In particular, the resulting stress strain measurements and displacement data are providing unprecedented detail of a fully 3D deformation field, including in situ damage propagation.

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Title: Mathematical and Numerical Modelling for Microbial Weathering in Rocks

Author(s): Hitoshi Matsubara, *U. Ryukyus*.

Microbes such as endolithic bacteria attach to exposed mineral surfaces in rocks, coat them with extracellular polymers, and bore into the host rock by solubilizing cementing mineral grains in their attempt to gain access to nutrients and energy. The weathering patterns by microbes are quite different from those by chemical reactions. In fact, these enigmatic microboring structures such as tubular and granular structures have been found in modern and ancient rocks weathered by microbes, whereas such morphological features cannot be observed in chemical weathered rocks. Although microbial contributions in various rock types, such as limestone, dolomite, sandstone, granite, basalt, etc. have been well documented based on petrographic and geochemical approaches to date, we may never obtain such microstructures in laboratory experiments with the traditional approaches because microboring structures caused by microbes in rocks may take hundreds of years to develop. In contrast, mathematical modelling and numerical simulation can circumvent the time issue, and as such, the application of various simulation patterns might be the much step forward in resolving the formation processes of microbial rock weathering. In this work, a novel mathematical model is presented for rock weathering by euendolithic bacteria. This model assumes that the bacteria employ a chemolithoautotrophic metabolism and have access to an infinite supply of nutrients via rock dissolution. As numerical examples, I show some simulation results for the formation process of the putative microfossils which may be the oldest morphological evidence for life on Earth. In this research, some numerical simulations are demonstrated, which are very similar to the microboring structures recorded in the ancient rocks.

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Title: Numerical Material Testing for FRP with a Finite Strain Viscoelastic-Viscoplastic Model

Author(s): Seishiro Matsubara, *Tohoku U.*; Kenjiro Terada, *Tohoku U.* .

The thermoplastic resins are known to exhibit different creep properties during their deformation process. Roughly classified, viscoelastic response is dominant at small or moderate strain regime, whereas viscoplastic behavior becomes prominent at large strain regime. Peculiar stress softening is observed just after the initial yielding and is followed by the transition to the viscoelastic and viscoplastic material responses prior to the final stress-buildup. At the same time, the material properties strongly depend on temperature so that material behavior is dramatically changed in the vicinity of the glass transition temperature. In addition, the material is melted by further temperature increase so as not to sustain further mechanical loading. In order to represent the above-mentioned complex mechanical behavior of thermoplastic resins, we propose a viscoelastic-viscoplastic combined constitutive model within the framework of finite strain thermodynamics with a view to application to two-scale analysis of fiber-reinforced plastics (FRP). Setting up a rheological model, different kinds of hyperelastic constitutive laws are used for the viscoelastic and viscopelastic rheological elements. A generalized Maxwell model is used to characterize the viscoelastic material behavior at small or moderate strain regime, while a finite strain viscoplastic model is employed to transient creep deformations due to frictional resistance of molecular chains. Also, back stress is introduced to represent the hardening due to orientation of molecular chains. After the fundamental performance of the proposed model is verified in representing typical material behavior of resin, representative numerical examples are presented to demonstrate the capability of the proposed model in reproducing the stress-softening, non-homogeneous creep, stress-buildup and self-heating phenomenon due to large inelastic deformations as well as the deformation-rate dependency. Then, the model is applied to the numerical material testing (NMT) for periodic microstructures (unit cells) of fiber-reinforced plastics (FRP) so that the overall anisotropic inelastic behavior is characterized based on the mathematical homogenization. In particular, we are concerned with the effect of self-heating behavior due to large strains distributed locally in a unit cell on the macroscopic mechanical behavior.

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Title: Multi-Scale Simulation of Advanced High Intensity-Focused Ultrasound Therapy

Author(s): Yoichiro Matsumoto, *U. Tokyo*.

High Intensity Focused Ultrasound (HIFU) therapy is one of the non-invasive cancer treatments, which provides the ablation of tissue around the focal point of ultrasound. HIFU therapy has been applied for the cancer close to the body surface such as the breast cancer and prostate cancer. The development of HIFU therapy for the deeply placed cancers, like liver and pancreas, are desired. Some problems are the displacement of the focal point due to the inhomogeneity in human body and the weak intensity of the sound pressure due to the long distance propagation. The objectives of present study are the realization of the appropriate focus control by an array transducer, the support of the preoperative planning of HIFU therapy by the prediction of ablation regions and the augmentation of the ablation effects by the injection of micro bubbles as an enhancer. The HIFU therapy with an array transducer for a liver cancer is reproduced numerically. A clear focal point is obtained at the target by the array transducer with the appropriate phase delay which is provided by the pre-computation of the ultrasound propagation from the target. The augmenting effect for the ablation by micro bubble injection is successfully confirmed by multiscale simulation for the bubbly media.

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Title: Uncertainty Quantification for Groundwater Contamination Using Measure Theory

Author(s): Steven Mattis, Clint Dawson, *UT Austin*; Troy Butler, *U. Colorado-Denver*.

The movement of contaminant plumes in underground aquifers is highly dependent on many hydrogeological parameters. Some of these parameters include porosity, flow direction, flow speed, dispersivities, and effects of geochemical reactions. It is often prohibitively expensive or impossible to make accurate and reliable measurements of these parameters in the field. It is also difficult to know the position and shape of a contaminant plume at a given time or the exact details of the source of the contamination, e.g. size, location, origin time, and magnitude. If decisions are to be made regarding contaminant remediation strategies or predictions of future contaminant concentrations in and near water-supply wells, then these uncertain hydrogeological and source parameters need to be analyzed and estimated. However, this is difficult with traditional methods due to the large number of uncertain parameters and relatively small amount of observable data. We utilize a measure-theoretic inverse framework to perform uncertainty quantification and estimation for these parameters. In this framework, we compute approximate solutions to inverse problems for determining parameters in models with stochastic data on output quantities. The formulation of the problem and modeling framework define a solution as a probability measure on the parameter domain for a given sigma-algebra. In the case where the number of output quantities is less than the number of parameters, the inverse of the map from parameters to data defines a type of generalized contour map. The approximate contour maps define a geometric structure on events in the sigma-algebra for the parameter domain. We utilize an inherently non-intrusive method of sampling the parameter domain and events in the given sigma-algebra to approximate the probability measure. We determine optimal quantities of interest (QoI) defining reduced-dimension set-valued inverses for this measure-theoretic inverse framework.

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Title: Using Workflow Provenance Data to Analyze Performance Data of Numerical Methods

Author(s): Renan Souza, Vitor Silva, Danilo Costa, Alvaro Coutinho, Marta Mattoso, *COPPE/Federal U. Rio de Janeiro*.

Computer simulations are usually performed by multiple combinations of programs, each of which has a set of parameters and input data. These simulations can be modeled as scientific workflows and managed by Scientific Workflow Management System (SWfMS). Parallel SWfMS are generic tools that can be used to encapsulate the parallelism of a parameter sweep exploration for different simulation codes. Another advantage of using SWfMS to manage a large-scale simulation is the improvement of resulting data analysis through provenance. Provenance data represents the workflow execution behavior, allowing for tracing back the generation of the data-flow. Provenance data becomes especially useful for users when execution behavior is clearly associated to corresponding domain data. Although several SWfMS provide sophisticated mechanisms for executing large-scale scientific workflows in distributed HPC environments, most of them execute the workflow in an “offline” way, as a black-box. Online monitoring and debugging may save significant amounts of workflow execution time, when unexpected behavior can be detected way before the end of the workflow execution. Provenance data is an important asset to identify and analyze errors or misconfigurations that occurs during the workflow execution (i.e. performance data analysis). This analytical process is fundamental for workflows that execute in parallel in large-scale distributed environments since the incidence of errors in this type of execution is high and difficult to track. In most of the executions, the debugging process has to explore the content of data files, iteratively searching for the identification of what caused the anomalous execution. Since each workflow execution may consist of hundreds or even thousands of tasks that are executed in parallel, it is unviable to perform a manual monitoring and debugging on data-flow generation. By querying the provenance repository, users have different ways to identify errors at runtime and take the necessary actions. We present our performance analysis experiences, based on provenance data, in real use cases of computational fluid dynamics and seismic imaging workflows. Users query provenance data to relate domain and execution data as a complement to Tau performance analyzer, especially when the execution concludes without any system error message.

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Title: Topology Optimization for 3D Printed Active Composites

Author(s): Kurt Maute, Anton Tkachuk, Markus Geiss, *U. Colorado*; Jiangtao Wu, Jerry Qi, *Georgia Inst. Technology*; Martin Dunn, *Singapore U. Technology & Design*.

Multi-material polymer printers allow the placement of different material phases within a composite, where some or all of the materials may exhibit an active response. Utilizing the shape memory behavior of at least one of the material phases, active composites can be 3D printed that deform from an initially flat plate into a curved structure. This paper introduces a topology optimization approach for finding the spatial arrangement of shape memory polymers within an inactive matrix such that the composite assumes a target shape. The optimization approach combines a level set method for describing the material layout and a generalized version of the extended finite element method (XFEM) for predicting the response of the printed active composite (PAC). This combination of methods yields optimization results that can be directly printed without the need for additional post-processing techniques. The response of the composite is described by two multi-physics models that differ in the level of accuracy of approximating of the residual strains generated by a thermo-mechanical programming process. Comparing XFEM predictions of the two PAC models against experimental results suggests that the models are sufficiently accurate for design purposes. The proposed optimization process is studied with examples with target shapes corresponding to a bending type deformation and to a localized deformation. The optimized designs are 3D printed and the XFEM predictions are compared against the experimental measurements. The design studies demonstrate the ability of the proposed optimization method to yield a crisp and highly resolved description of the optimized material layout that can be realized by 3D printing. As the complexity of the target shape increases, the optimal spatial arrangement of the material phases becomes less intuitive, highlighting the advantages of the proposed optimization method.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: An Hp-Adaptive Anisotropic Meshing Technique for Convection-Diffusion Problems

Author(s): Georg May, Aravind Balan, Michael Woopen, *RWTH Aachen U.*.

We present a novel anisotropic hp mesh adaptation technique for numerical solution of linear and nonlinear partial differential equations. Focus is in particular on convection-diffusion problems, including the compressible Euler and Navier-Stokes equations. Our approach is compatible with general numerical methods using piecewise polynomial solution representation. In many engineering applications, one is often primarily interested in some specific solution-dependent output functional. In aeronautical applications, examples are given by lift and drag coefficients. Our aim is to generate meshes for the numerical solution of a PDE problem, which are optimal, or near optimal, with respect to a given output functional. The approach combines an adjoint-based goal-oriented error estimator with an optimization of the anisotropy of mesh elements using metric-based mesh manipulation. New meshes are created from an optimized metric map at each adaptation step using a metric-based mesh generator [1]. This process takes into account both solution features and error distribution with respect to the target functional: The isotropic size of the mesh is decided by the adjoint error estimator and the optimal anisotropy is determined by minimizing the interpolation error in a constrained piecewise polynomial approximation space. The overall approach, including an hp extension which optimizes the local polynomial degree of approximation, is a further development of the approach presented in [2], incorporating our adjoint-based error estimate. We present validation using finite element methods on triangular grids for various test cases, including scalar model equations, as well as inviscid transonic, supersonic and laminar viscous flow around the NACA0012 airfoil. [1] F. Hecht. Bamg: Bidimensional anisotropic mesh generator. Technical report, INRIA-Rocquencout, France, 2006. [2] V. Dolejsi. Anisotropic hp-adaptive method based on interpolation error estimates in the lq-norm. Applied Numerical Mathematics, 82:80–114, 2014

13th U.S. National Congress on Computational Mechanics
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Title: Enhancing the Efficiency and Robustness of Monolithic Fluid-Structure Interaction Solvers

Author(s): Matthias Mayr, Wolfgang A. Wall, Michael W. Gee, *Tech. U. München*.

Solving incompressible fluid-structure interaction problems numerically still poses a computationally challenging problem. Monolithic solvers as proposed in [1,2] have proven to be very robust and efficient and have been shown to outperform partitioned approaches by far for certain very demanding FSI cases. Various essential ingredients are required to apply these types of algorithms to large scale sophisticated examples. Some of them are parallel hardware and software architecture, adaptive time stepping procedures based on error indication, FSI-specific linear preconditioners [3] and special nonlinear solution techniques to name a few. Recent progress has been made in applying adaptive time stepping procedures in order to obtain time-accurate results with reasonable computational costs. In addition, the application of special nonlinear solution techniques, that avoid solving the monolithic linear systems like in a Newton-type fashion, seems to be very promising, especially when it comes to very large system sizes on massively parallel machines. In the presentation, we will detail recent advances in tackling the above mentioned issues and discuss some of the key ingredients to obtain performant monolithic solvers for FSI problems. We compare our approach to existing methods. Examples will be provided that demonstrate the behaviour of the newly proposed methods with respect to accuracy, computational costs, and computational savings. [1] Mayr, M., Klöppel, T., Wall, W.A., Gee, M.W. (2015): A Temporal Consistent Monolithic Approach to Fluid-Structure Interaction Enabling Single Field Predictors, SIAM Journal on Scientific Computing, 37(1), B30-B59 [2] Heil, M. (2004): An efficient solver for the fully coupled solution of large-displacement fluid-structure interaction problems, Computer Methods in Applied Mechanics and Engineering, 193(1-2), 1-23 [3] Gee, M.W., Küttler, U., Wall, W.A. (2011): Truly monolithic algebraic multigrid for fluid-structure interaction, International Journal of Numerical Methods in Engineering, 85(8), 987-1016

13th U.S. National Congress on Computational Mechanics
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Title: The Principle of Stationary Action and Fundamental Solutions of Two-Point Boundary Value Problems

Author(s): William McEneaney, *UC San Diego*; Peter Dower, *U. Melbourne*.

Two-point boundary value problems (TPBVPs) for conservative systems are studied in the context of the stationary action principle. In particular, we consider the case where the initial boundary condition is the system position, and the terminal boundary condition may be a combination of position and velocity data. We specifically consider the wave equation and the n-body problem. An object is obtained which functions as a fundamental solution. Specifically, once one computes this fundamental solution, one may obtain solutions for a variety of boundary conditions without re-propagation over time. In the case of the wave equation, the fundamental solution is obtained as a solution of an infinite-dimensional differential Riccati equation, and solution of the TPBVP for varying boundary data is obtained through max-plus convolutions of the fundamental solution with functions related to that boundary data. In the case of the n-body problem, there is an additional idempotent convolution required beyond the one for the wave equation. This additional convolution is required because the gravitational potential is represented via convex duality. This duality-based representation leads to a differential game representation, where the inner player is solving a linear-quadratic control problem. In this case, the fundamental solution is a convex set in a finite-dimensional space, where the set consists of solutions of differential Riccati equations.

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Title: Spacetime Simulation of Seismic Response

Author(s): Ian McNamara, Robert Haber, Ahmed Elbanna, *U. Illinois, Urbana-Champaign*; Reza Abedi, *U. Tennessee Space Inst.* .

Analytical and numerical investigations of the dynamic behavior of faults has generated new insights into the mechanics of seismic response, including for example, intersonic fracture [1] and the role of velocity-weakening friction in determining whether the rupture mode is self-healing or crack-like [2]. Numerical simulation provides an important complement to observational, experimental, and analytical investigations, due to its ability to model complex configurations and reveal details of response that are not easily measured in the field or laboratory. However, dynamic, frictional contact and rupture are still challenging problems in numerical simulation, especially when high-fidelity models suitable for scientific investigation are needed. We present an adaptive, spacetime discontinuous Galerkin finite element model for seismic research, adapted from previous work on engineering fracture mechanics [4], that we hope meets these requirements. We include a contact model with slip-weakening friction that enforces Riemann conditions to preserve the characteristic structure of the underlying elastodynamic system. An interfacial damage model, supported by powerful mesh adaptation and a stochastic nucleation criterion, represents mode-II fracture in simulations of fault branching and roughening. We present numerical results to demonstrate the spacetime model's capability for high-resolution simulation of seismic physics, and discuss prospects for supporting more sophisticated friction models, such as rate and state-based models with enhanced weakening, in the SDG framework. References [1] Rosakis, A. J., O. Samudrala and D. Coker, 1999. Cracks Faster than the Shear Wave Speed. Science 284, 1337–1340. [2] Zheng. G. and J. R. Rice, 1998. Conditions under which Velocity-Weakening Friction Allows a Self-healing versus a Cracklike Mode of Rupture. Bull. Seismological Soc. Am. 88, 1466–1483. [3] Abedi, R. and R. B. Haber, 2014. Riemann solutions and spacetime discontinuous Galerkin method for linear elastodynamic contact. Comput. Methods Appl. Mech. Engrg. 270, 150–177.

13th U.S. National Congress on Computational Mechanics
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Title: Modeling Fluid-Structure Interaction Using Energy Finite-Element Analysis for Bounded and Unbounded Fluid Domains

Author(s): Sergey Medyanik, *Michigan Engineering Services, LLC*; Nickolas Vlahopoulos, *U. Michigan*.

Fluid-structure interaction problems that involve vibration at mid-to-high frequencies can be conveniently studied using Energy Finite Element Analysis (EFEA) which provides superior computational efficiency compared to conventional finite element methods. Standard Finite Element Analysis (FEA) methods solve differential equations for which the fundamental solutions vary harmonically with space, thus the wavelength becomes smaller as the frequency increases requiring a prohibitively large number of elements and computational resources. In the EFEA method, the governing differential equations are formulated for an energy density variable that has been spatially averaged over a wavelength and time averaged over a period. The corresponding fundamental solutions vary exponentially with space, thus requiring only a small number of elements to capture the smooth spatial variation. Coupling between structural and fluid domains is achieved in EFEA through the joint matrices that govern the flow of energy between the different parts of the system. Standard Galerkin formulation is typically applied in EFEA for modeling bounded reverberant structural and fluid domains. In this case the corresponding differential equations are self-adjoint and Galerkin formulation yields a stable solution. However, for unbounded non-reverberant domains the resulting differential equations have non-self-adjoint part and Galerkin formulation leads to unstable oscillatory solutions. Instead, a stabilized approach, such as Streamline Upwind Petrov-Galerkin (SUPG), must be employed in order to resolve the oscillatory behavior. In this work, the stabilized finite element method will be applied to unbounded fluid domains that are either independent or coupled with structures that are modeled using standard Galerkin FEM. Differences in modeling bounded and unbounded fluid domains in EFEA will be outlined. Theoretical aspects of the new formulation will be discussed and results of numerical simulations will be presented and validated by comparing to closed form analytical solutions as well as experiments.

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Title: Regularizing the Inverse Problem to Solve the Elastic Property Distribution of Vascular Tissues

Author(s): Yue Mei, Sevan Goenezen, *Texas A&M U.*.

Vascular tissue diseases, such as atherosclerotic plaques, intracranial aneurysms, or abdominal aortic aneurysms, can be detected via medical images from intravascular ultrasound, magnetic resonance imaging (MRI), or computed tomography (CT) scan. An alternative and more recent approach to detect diseased tissues, utilizes images of the elastic property distribution, which is more commonly known as elasticity imaging or elastography. In these images, diseased tissues can be distinguished from healthy tissues based on their stiffness contrast. This can be done as diseased vascular tissues change their microstructure, e.g., increasing their collagen fiber content, elastin degradation, etc., which alters the tissue's macroscopic material behavior. The elastic property distribution is determined from the solution of an inverse problem in elasticity for which we require the knowledge of the displacement field of the vascular tissues. The displacement field can be determined from medical images, acquired while the vascular tissue domain of interest is deformed, e.g., passive deformation due to expansion and contraction during the systolic and diastolic cardiac cycle. In this presentation we discuss the solution of the inverse problem in elasticity for the shear modulus distribution on a hypothetical atherosclerotic plaque study. The vulnerable plaque is described as a large and soft lipid, covered by a thin cap. In our model, the intraluminal pressure at systole and diastole are prescribed as boundary conditions, causing the deformations in the subsurface vascular tissue walls. We solve the inverse problem as a constrained minimization problem subject to the constraint of the equations of equilibrium. In the objective function, we minimize the displacement correlation between measured and computed displacements under Tikhonov regularization, where the computed displacement field satisfies the equations of equilibrium for the current estimate of the shear modulus distribution. We use finite element algorithms to discretize and solve the inverse problem. We will show that the particular choice of regularization is crucial to successfully solve the inverse problem in elasticity in the presence of high noise levels in the displacement data. To this end, we introduce a novel regularization type, having sophisticated properties as compared to alternative regularization methods.

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Title: A Finite Element Model for Arbitrarily Oriented Fibers and their Contact Interaction Based on Geometrically Exact Kirchhoff Beam Elements

Author(s): Christoph Meier, Alexander Popp, Wolfgang A. Wall, *Technische U. München* .

In countless applications ranging from classical engineering (e.g. cables, composites) to biophysics (e.g. biopolymer networks) mechanical system performance is determined by highly slender, fiber-like components which can be described as 1D-Cosserat continua. In all these examples, contact interaction crucially influences the overall system behavior. We propose a geometrically exact Kirchhoff formulation tailored to deal with the high slenderness ratios of such fibers and related numerical challenges such as locking or ill-conditioning. Moreover, in some of these systems, the influence of torsion is negligible. We address this special problem class by additionally providing a torsion-free variant of the proposed Kirchhoff element which can completely abstain from rotational degrees of freedom and related complexities without losing desirable properties such as the high accuracy and efficiency of geometrically exact beam formulations. The proposed elements are based on a C1-continuous Hermite interpolation enabling smooth contact kinematics. The second core component of our simulation framework is an efficient and robust contact algorithm. Most state-of-the-art beam-to-beam contact formulations are of point-to-point contact type [1]. While providing a very efficient, consistent and easy-to-implement contact algorithm, this procedure fails for configurations that consist of almost parallel beams enclosing small angles. Alternative formulations also enable the treatment of small contact angles [2]. However, these formulations typically require a beam slenderness-dependent, very fine, and therefore expensive contact discretization to resolve beam-to-beam contact in the range of large contact angles. Our approach is based on a combination of the advantages of both types of formulations. We apply a point-to-point contact formulation in the range of large contact angles. The scope of small contact angles is covered by a line-to-line contact formulation. The model-transition between these two formulations within a prescribed angle interval is realized in a variationally consistent manner. Furthermore, all configuration-dependent quantities describing the point-contact, the line-contact and the transition-contact range are consistently linearized, thus allowing for an application within the framework of implicit time integration. [1] Wriggers, P. and Zavarise, G., “On contact between three-dimensional beams undergoing large deflections”, Communications in Numerical Methods in Engineering, 13, 429-438 (1997). [2] Durville, D., “Simulation of the mechanical behaviour of woven fabrics at the scale of fibers”, International Journal of Material Forming, 3, 1241-1251 (2010). [3] Meier, C., Popp, A. and Wall, W. A., “An objective 3D large deformation finite element formulation for geometrically exact curved Kirchhoff rods”, Computer Methods in Applied Mechanics and Engineering, 278, 445-478 (2014).

13th U.S. National Congress on Computational Mechanics
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Title: Transient Impinging Jet in Crossflow as a Benchmark Case to Validate Unsteady LES

Author(s): Hubert Baya Toda, *IFP-Energies Nouvelles*; Olivier Cabrit, *U. Melbourne, Australia*; Karine Truffin, Gilles Bruneaux, ; Simon Mendez, Franck Nicoud, *U. Montpellier*.

Computational Fluid Dynamics (CFD) is more and more used in the context of cardiovascular biomechanics, to predict blood flows in physiological and non-physiological conditions. However, compared to other fields in Mechanical Engineering, cardiovascular CFD has some specific features: blood is a complex fluid, boundary conditions (geometries and flow conditions) are sometimes poorly known, fluid-structure interaction is often present. In addition, the flow may be pulsatile with a transitional regime, between laminar and fully turbulent. This reason motivates more and more groups to use large-eddy simulations (LES). There is thus a growing interest for relevant benchmark cases: the interest for CFD has notably led the U.S. Food & Drug Administration to initiate the “FDA Critical Path Initiative” to evaluate the use of CFD in the design of cardiovascular devices. In its First Computational Interlaboratory Study1, a cylindrical nozzle with a conical collector and sudden expansion on either side of a throat was considered to assess the ability of CFD to capture the transition to turbulence after the sudden expansion. However, such a case is stationary, and may be sensitive to slight changes in the numerics and to inlet flow disturbances. Here, we present an experimental database2 designed for the validation of CFD, and in particular of LES. The configuration is a pulsatile jet in a turbulent cross-flow impinging on a plate. The case of a pulsatile jet interacting with a wall is actually typical of the early diastole in the human left ventricle, when the E wave vortex ring interacts with the lateral wall3. In addition, this case has the advantage of gathering many selective aspects for turbulence and turbulence transition simulation. The crossflow is turbulent and bounded by a plate, on which a turbulent boundary layer develops. The unsteady jet generates a large laminar vortex ring that impacts on the plate, generating smaller vortices. After the impact, the main vortical structure is transported by the crossflow along the plate. All these different aspects are crucial for the quality of a simulation. In addition to the experimental database, we will present results of numerical simulations for different eddy-viscosity models2. [1] S.F.C. Stewart et al. Cardiovascular Engineering and Technology, 3(2), 2012 pp. 139–160 [2] H. Baya Toda, O. Cabrit, K. Truffin, G. Bruneaux, F. Nicoud. Physics of Fluids, 2014, 26, 075108. [3] C. Chnafa, S. Mendez, F. Nicoud. Computers and Fluids, 2014, 94, pp 173-187.

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Title: Evaluation of Electronic Transport Across Grain Boundaries in Graphene

Author(s): Juan Pedro Mendez, M. Pilar Ariza, *U. Seville*; Michael Ortiz, *Caltech*.

In the field of electronics, due to its excellent mechanical and electrical properties, graphene has become the most promising material for the production of next generation electronic components. However, with all the research findings up to date, owing to the fact that defect-free graphene presents a lack of band gap, it is well known the limited use of this material for semiconductor-based applications, such as field effect transistors. Many attempts have been successfully made to engineer band gaps in graphene, such as doped or uniaxial strained membranes and manufactured nanoribbons. In this work, we focus on a new innovative way to introduce relevant transport gaps in graphene associated with the existence of asymmetrical grain boundaries in the lattice. First, we have identified stable grain boundary structures by recourse of a computational tool based on the Landauer-Büttiker formalism [1]. The electronic transport across these grain boundaries is then evaluated based on a tight binding model. In addition, in order to validate our results against ab initio-based calculations, we have also employed the density functional formalism and the non-equilibrium Green's function method implemented in TRANSIESTA code [2,3]. As main result, we have found that some asymmetric grain boundary structures provide a moderate transport gap, up to ~ 1eV. [1] Datta, S. (1995). Electronic Transport in Mesoscopic Systems. Cambridge University Press, Cambridge. [2] Soler, J.M et al. The siesta method for ab initio order-n materials simulation. Journal of Physics: Condensed Matter, 14, 2745. [3] Brandbyge, M. et al. (2002). Density-functional method for nonequilibrium electron transport. Phys. Rev. B, 65, 165401.

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Title: On Godunov-Type Methods for Computing Compressible Two-Phase Flows

Author(s): Igor Menshov, *KIAM RAS, VNIIA ROSATOM*.

In the present paper we consider numerical methods for solving compressible two-phase Euler equations. The model to be used is a modification of that of Baer-Nunziato and serves to describe non-equilibrium flows of a dispersed gas-solid medium. We aim to develop a Godunov-type approach to discretizing the system of governing equations on an arbitrary moving Eulerian grid. To do this, we follow the method of splitting in physics and first divide the problem into two sub-problems for dynamics of (1) the solid phase and (2) the gas phase in the solid skeleton, respectively. The equations (1) govern the change of the solid volume fraction, and other solid parameters. This is not strictly hyperbolic system as the solid (intergranular) pressure vanishes when the volume fraction becomes less than a critical value (closed-packed structure). We formulate the non-linear Riemann problem for the solid equations and find its exact solution under minor assumptions. The numerical flux is then approximated with the solution obtained. The resulting scheme is shown to be able to work correctly in all the region of the volume fraction change. For the equations (2) we first develop the Rusanov method that was applied in [1] to solve numerically the non-conservative Euler equations with fixed (in time) porosity function. First, we show how to extend the standard (uniform porosity) Rusanov method to moving Eulerian grids. Then this approach is generalized for the case of non-conservative (variable porosity) equations. We formulate the property of well-balanced scheme for the moving grid case and prove that the generalized Rusanov flux possesses this property. Finally, with the use of the technique described in [2] we propose a well-balanced Rusanov scheme for the non-conservative equations with the porosity changed both in space and in time. For the equations (2) we also discuss the non-linear Riemann problem. Its solution involves an iterative procedure of solving a couple of non-linear equations for pressures at the discontinuity of porosity. The accuracy and robustness of the proposed method is demonstrated in numerical calculations of several test problems (a kind of Sod problems in porous moving medium) that have exact solutions. As an application we intend to show calculations of granular explosives detonation. References. [1] S. Clain, D. Rochette. JCP, 228, 2009, 8214-8248. [2] I. Menshov, A. Serezhkin. ECCOMAS Proceedings, 2014.

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Title: On an Application of a Continuum Homogenization Theory to Materials Under High-Frequency Dynamic Loading

Author(s): Brian Mercer, Panayiotis Papadopoulos, Kranthi Mandadapu, *UC Berkeley*.

This talk presents a general theory that addresses homogenization of material behavior under high-frequency loading. The theory [1] is derived using an approach similar to that of Irving and Kirkwood [2] for calculating continuum quantities, such as stress and heat flux, from atomistic variables. As in the atomistic formulation, the continuum version of the theory shows that there is a kinetic contribution to the macroscopic stress that involves velocity fluctuations about the mean; as the magnitude of these fluctuations increases, so does their influence on the overall macroscopic stress. As such, the theory is particularly relevant to dynamic loading that produces wavelengths on the order of, or smaller than, the characteristic length scales of the material microstructure. By way of a canonical example, we consider the problem of one-dimensional periodically layered elastic media subject to dynamic loading, and explore the range of frequencies for which the kinetic stress makes a significant contribution to the total macroscopic homogenized stress. In addition, we show that typical FE2 homogenization methods are not suitable for solving problems involving wavelengths on the order of the material length scale, since the these waves cannot be accurately resolved and propagated on the coarser macroscopic finite element mesh. Practical applications and implications of the theory are also discussed. References: [1] Mandadapu, K.K., Sengupta, A., Papadopoulos, P. A homogenization method for thermomechanical continua using extensive physical quantities. Proc. R. Soc. A., 486, pp 1696--1757, 2012. [2] Irving, J.H., Kirkwood, J.G. The statistical mechanical theory of transport processes. IV. The equations of hydrodynamics. J. Chem. Phys., 18, pp. 817--829, 1950.

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Title: The Insertion of a Submesh with the Extended Finite-Element Method

Author(s): Mark Merewether, Tim Shelton, Mike Veilleux, *Sandia Nat'l. Lab.*; John Dolbow, *Duke U.*.

With the ever advancing capabilities within the eXtended Finite Element Method (X-FEM) to model complex crack growth and branching, a need has arisen to robustly keep track of the cuts in a single element. When a single element contains two or more cracks, the bookkeeping can become very complicated. We propose the use of an X-FEM submesh to handle this algorithmically challenging problem. With the use of the submesh, we will show that we are able to conserve the mass of the original problem even with these complex crack patterns. We will also demonstrate our ability to realistically capture fragment distributions. In addition to the simplified bookkeeping and mass conservation, the submesh also provides an easy mechanism for creating contact surfaces on the new cut geometry. With the contact surfaces in place, we are able to model an important suite of problems where both fragmentation and contact play significant roles such as the blast loading of structures. Prepared for the 13th US National Congress on Computational Mechanics, July 26-30, 2015 San Diego, CA, USA. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: An MBO Scheme on Graphs for Classification and Image Processing

Author(s): Ekaterina Merkurjev, Andrea Bertozzi, *UCLA*; Tijana Kostic, *Microsoft*; Allon Percus, *Claremont Grad. U.*; Arjuna Flenner, *NAVAIR*; Cristina Garcia-Cardona, *LANL*.

In this talk, we present a computationally efficient algorithm utilizing a fully or semi nonlocal graph Laplacian for solving a wide range of learning problems in data classification and image processing. In their recent work "Diffuse Interface Models on Graphs for Classificaiton of High Dimensional Data", Bertozzi and Flenner introduced a graph-based diffuse interface model utilizing the Ginzburg-Landau functional for solving problems in data classification. Here, we propose an adaptation of the classic numerical Merriman-Bence-Osher (MBO) scheme for minimizing graph-based diffuse interface functionals, like those originally proposed in the paper by Bertozzi and Flenner. A multiclass extension is introduced using the Gibbs simplex. We also make use of fast numerical solvers for finding eigenvalues and eigenvectors of the graph Laplacian, needed for the inversion of the operator. Various computational examples on benchmark data sets and images are presented to demonstrate the performance of our algorithm, which is successful on images with texture and repetitive structure due to its nonlocal nature. Image processing results show that our method is multiple times more efficient than other well known nonlocal models. Classification experiments indicate that the results are competitive with or better than the current state-of-the-art algorithms.

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Title: Parallel Scalable Anisotropic Adaptation for Fluid-Structure Interaction

Author(s): Youssef Mesri, Elie Hachem, *Mines Paristech*.

This work is motivated by the potential of both the adaptive and stabilized finite element methods in accurately simulating complex industrial physical systems in science and engineering. Indeed, we will show that the use of immersed volume methods to deal precisely with complex geometries combined with advanced finite element solvers to handle unsteady turbulent flow simplifies setting fluid-structure interaction simulations in a parallel framework. Moreover, we propose an anisotropic a posteriori error estimator that controls the error due to mesh discretization in all space directions. The obtained optimal metric is then used to build the optimal mesh and also to derive an efficient scalability model. However, these advances are challenging in a parallel runtime execution for which we should take into account the dynamic aspect of the parallel remeshing (domain discretization). The parallel remeshing involves parallel mesh repartitioning in order to load balance the global workload and reducing interface communications. Therefore, several tools and algorithms were developed and optimized in the last years to overcome such challenges and to prepare them towards exascale computing. A leading question arises after all from this analysis: how to derive a scalability model to measure the parallel efficiency of our adaptive simulation code? Indeed, it is complicated today to derive a model of performance of dynamic parallel finite element meshes. The mesh adaptation procedure changes dynamically the size of the mesh over all the processes. In other words, the size of the problem changes permanently along the runtime execution. Different answers and scalability studies demonstrating the effectiveness of our methods on several 3D industrial fluid-structure interaction problems will be presented.

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Title: Anisotropic Mesh Adaptation for Cracks in Brittle Materials with Phase-Field Methods

Author(s): Stefano Micheletti, Simona Perotto, Nicola Ferro, Marianna Signorini, *Politecnico di Milano*.

In this communication we are concerned with the numerical simulation of fractures in brittle materials under a quasi-static approximation. Several are the configurations where cracks form and propagate, typically in the fields of civil and mechanical engineering. For example, the shrinkage of materials, induced by a thermal shock due to sudden cooling or drying, may lead to arrays of regularly spaced cracks. The detection of these cracks is of crucial importance as they can weaken the body and sometimes compromise its safety. In other circumstances, geometrical features in the material, e.g., holes and slits, can facilitate the onset of fractures and influence their propagation under loading. A very accurate variational model for quasi-static brittle fractures is Francfort-Marigo's, which involves the minimization of a highly irregular energy functional. A suitable approximation of this model, based on Gamma-convergence, can be obtained by the Ambrosio-Tortorelli functional. In this case, the crack is identified by a smooth phase-field, instead of a lower-dimensional set, as in the Francfort-Marigo model. An efficient approach to the numerical solution of the adopted variational problem relies on mesh adaptation, possibly driven by an a posteriori error estimator, in order to refine the grid only in a thin neighborhood of the crack path. In [1,2], an anisotropic a posteriori error estimator and a new minimization algorithm are proposed and applied to the classical Ambrosio-Tortorelli approximation, in the case of both anti-plane and plane-strain isotropic linear elasticity. The employment of an anisotropic grid allows one to considerably reduce the number of mesh elements in comparison with a corresponding isotropic adaptation technique, and thus to save on the overall computational cost. In this communication, we extend the approach presented in [1,2] to the generalized Ambrosio-Tortorelli model considered in [3], which allows one to deal with several types of brittle materials and more general variational models. [1] M. Artina, M. Fornasier, S. Micheletti and S. Perotto, Anisotropic mesh adaptation for crack detection in brittle materials, Mox-Report, 20/2014. [2] M. Artina, M. Fornasier, S. Micheletti and S. Perotto, The benefits of anisotropic mesh adaptation for brittle fractures under plane-strain conditions. To appear in New Challenges in Grid Generation and Adaptivity for Scientific Computing, SEMA SIMAI Springer, Vol. 5, Springer Milano, S. Perotto, L. Formaggia Eds. (2015). [3] S. Burke, C. Ortner and A. Suli, An adaptive finite element approximation of a generalized Ambrosio-Tortorelli functional, Math. Models Methods Appl. Sci., 23(9), pp. 1663-697, (2013).

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Title: Data Driven Inverse Multi-Scale Design of Materials

Author(s): John G. Michopoulos, *Naval Rsch. Lab.*.

An overview of a framework for designing materials that satisfy specific data-driven performance requirements, is presented. Three examples will be presented, two at the opposite ends of the length scale spectrum and one spanning various scales. In the atomistic scale level the determination of the Lenard-Jones (L-J) potential parameters is presented for the case of the dynamics of a problem of fracture such that a specific load history of the associated medium is satisfied. The problem is expressed as an inverse problem. A global Monte Carlo optimizer along with a molecular dynamics code are implemented to compute the L-J constants. In the macro scale the determination of a general set of material parameters that define the elastic and inelastic constitutive response of an anisotropic medium made from fiber-epoxy composite material laminates is presented. The specification requirements are the load-displacement histories in the full 6+6 dimensional kinematic space. A custom-developed recursive 6-DoF robotic loader was used to collect the actual kinematic responses of an existing material system. The determination of the material constants is achieved by minimizing objective functions such as the difference between experimentally measured and analytically computed system responses as described by strain fields and surface strain energy densities. Examples based on both synthetic and actual data demonstrate the successful constitutive characterization. In the multiscale context the application of an inverse methodology is demonstrated for identifying material properties of the constituents in the micro-scale of a selected composite material by utilizing macro-scale based experimental data. Taking advantage of a computational homogenization technique for periodic microstructures, the proposed optimization methodology allows for the determination of a considerable number of the elastic properties of the composite material at the micro-scale. The theoretical development and numerical implementation of a multi-scale modeling chain of the composite is presented, extending from the periodic microstructure represented by a suitable unit cell and subjected to appropriate periodic boundary conditions at the micro scale, up to the composite lamina at the meso-scale, to the laminated, multi-axially loaded material at the macro-scale. By applying the proposed methodology, several fiber and matrix properties have been calculated by utilizing properly generated synthetic data of the macro-scale behavior of the composite laminate. Furthermore, in an effort to explore the potential of the proposed method for identifying quantities that manifest after manufacturing, an effort has been initiated to determine fiber-matrix interfacial properties that has led to initial success.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Blended Isogeometric-Discontinuous Galerkin Methods for Multiphysics Applications and Shape Optimization

Author(s): Craig Michoski, John Evans, Luke Engvall, *U. Colorado-Boulder*; Jesse Chan, *Rice U.*.

Discontinuous Galerkin (DG) methods provide robust numerical solutions that are not only high-order accurate and locally adaptable, but also enjoy unique performance features well-suited to contemporary HPC architectures. While maintaining high-order accuracy over complex geometries can be achieved by warping curvilinear meshes using isoparametric mappings, this approach ultimately results in an approximate geometric representation. This is often of little consequence in single-physics applications, but can be undesirable in the multi-physics context -- such as in fluid-structure interaction where geometrically conforming approaches are required to enforce kinematic constraints between single-physics subsystems. This is of even greater concern in shape optimization wherein the derivative of the simulation with respect to the underlying Computer Aided Design (CAD) geometry must be computed. To address these concerns, we present a novel blending technique that leverages the relative strengths of DG methods with those of isogeometric analysis. The work is motivated by fluid-structure interaction problems, where nodal DG methods are used for the fluid subproblem and isogeometric analysis for the structural subproblem. To preserve geometric exactness in the volumetric fluid mesh along the fluid-structure interface, nodal DG elements are equipped with a superparametric rational Bezier mapping able to exactly parametrize the underlying CAD description of the interface. Using this blending method, exact geometry is preserved while simultaneously maintaining stability, accuracy, and efficiency features of standard nodal DG. This blending method further enables for evaluation of precise discrete shape sensitivities, which we demonstrate with a shape optimization example.

13th U.S. National Congress on Computational Mechanics
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Title: Effective Thermal and Elastic Properties of a Composite with Spheroidal Inhomogeneities

Author(s): Yozo Mikata, *Bechtel*.

This presentation will discuss the effective material properties of a composite with spheroidal inclusions and in particular voids. The method is based on Eshelby's equivalent inclusion method. Both dilute approximation and Mori-Tanaka's method will be discussed for disks, oblate spheroids and prolate spheroids, whose orientation is either aligned or completely random. Analytical formulations and numerical results will be given. In numerical results, all the constituents are assumed to be isotropic.

13th U.S. National Congress on Computational Mechanics
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Title: Structure-Property Modeling for the Heat Affected Zone in Linepipe Steels

Author(s): Matthias Militzer, *U. British Columbia*.

The integrity of pipelines depends critically on the quality of girth welds, in particular the properties for the heat affected zone (HAZ). In the HAZ the steel undergoes a rapid heat treatment during welding resulting in a graded microstructure that can be significantly different from that of the base metal. We have investigated a range of simulated HAZ thermal paths and welding scenarios for a state-of-the-art X80 linepipe steel in the laboratory to quantify the resulting microstructures and mechanical properties. Based on the experimental results microstructure-property models have been developed. Both the state variable approach and phase field modeling have been employed to model austenite grain growth and austenite decomposition into ferrite and bainite. The mechanical properties have been correlated with the grain size and dislocation density in the ferrite-bainite microstructure using a seamless approach accounting for the gradual transition from polygonal to irregular ferrite and bainite throughout the HAZ.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: An ALE-FEM for a Poroelastic Mixture Model for Fluid Flow in the Brain

Author(s): Scott Miller, Francesco Costanzo, *Penn. State U.*.

The lymphatic-like circulation in brain consists of cerebral spinal fluid (CSF) being drawn into arterial paravascular space from the arachnoid compartment, and subsequently cleared through the venous paravascular space. The term glymphatic has been coined to refers to this circulation system [1]. We are specifically concerned with modeling the cardiac-pulsation-driven CSF flow in the paravascular space of penetrating arteries and within the tissue around them. As this flow is driven by arterial wall motion it is inherently a fluid-structure interaction problem. We consider a model due to to Costanzo et al. in which brain tissue is viewed as an incompressible hyperelastic solid skeleton saturated by an incompressible fluid. The model is based on classical mixture theory [2] and is has distinct velocity fields for the fluid and the solid. There are four governing equations: the balance of mass for the constituents subject to the constraint that the sum of the volume fractions be equal to one; two equations for the balance of momentum of the fluid and the mixture, respectively; and a displacement-velocity kinematics relation for the solid skeleton. These equations are written in the reference configuration of the solid and, as such, they represent an application of an Arbitrary Lagrangian Eulerian approach. We have developed a mixed Galerkin ALE-FEM formulation with four primary fields: the pore pressure, the velocities of the fluid and solid, and the displacement of the solid skeleton. The formulation is unique in the manner in which integration by parts is selectively applied to ensure stability of the method. Time integration is performed with a theta-scheme similar to that in [3]. We present results illustrating the stability and convergence properties of the method, as well as notional simulations of peristaltic waves traveling along arteries. References [1] J. J. Iliff, H. Lee, M. Yu, T. Feng, J. Logan, M. Nedergaard, and H. Benveniste. Brain-wide pathway for waste clearance captured by contrast-enhanced MRI. The Journal of Clinical Investigation, 123(3):1299–1309, 2013. [2] R. A. Bowen, Incompressible porous media models by use of the theory of mixtures, International Journal of Engineering Science, 18 (1980), pp. 1129–1148. [3] T. Wick, Fluid-structure interactions using different mesh motion techniques, Computers and Structures, 89 (2011), pp. 1456–1467.

13th U.S. National Congress on Computational Mechanics
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Title: Computational Study of the Directed Self-Assembly of Porous Thin-Film Membranes with Colloidal Particle Coated Channels

Author(s): Paul Millett, Joseph Carmack, *U. Arkansas*.

Using a hybrid Brownian Dynamics-Cahn Hilliard (BD-CH) mesoscale computational approach, the coupled morphology of an immiscible binary polymer blend with dispersed colloidal particles is investigated in a confined thin-film geometry under the influence of an applied electric field. When the blend ratio is asymmetric (e.g. 30-70), the resulting microstructure consists of columnar channels of the B-phase perpendicular to the major plane of the film (aligned with the electric field), with the particles segregated along the channel interfaces. Upon selective dissolution of the minority phase, the channels will become pores with partially exposed colloidal particles that can react with an external fluid. This talk will focus on the computational results that illustrate the relationships between the average channel diameter, the channel areal density, and the interfacial particle packing fraction with varying particle number density and polymer blend ratio. Also of interest, the particles assume a hexagonal close-packed arrangement on the channel interfaces, although with a tilted helical angle that increases with decreasing channel diameter.

13th U.S. National Congress on Computational Mechanics
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Title: Optimization of the Parametric Design of a Bioprosthetic Heart Valve Based on Isogeometric Analysis

Author(s): Joshua Mineroff, Chenglong Wang, Baskar Ganapathysubramanian, Ming-Chen Hsu, *Iowa State U.*.

The goal of this research is to develop a framework to allow the efficient interface of optimization with isogeometric analysis (IGA) for the purpose of prosthetic heart valve design. IGA enables the effects of decisions to be quantified more seamlessly throughout the design process; besides refinement of the final geometry, optimization can also add value by suggesting directions for improvement. Pareto optimal geometries and material properties of a parametrically-generated bioprosthetic heart valve are identified using a dynamic simulation of the heart valve closure to calculate principal strain and coaptation area, a measure of prosthetic heart valve performance. We investigate the application of gradient-based and evolutionary-based methods to IGA, as well as the robust optimization of uncertain material properties.

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Title: Formability of Aluminum Alloys at Elevated Temperatures Using a New Thermo-Elasto-Viscoplastic Crystal Plasticity

Author(s): Raja K. Mishra, *General Motors* ; Ed Cyr, Mohsen Mohammadi, Kaani Inal, *U. Waterloo*.

In this paper, a new thermo-elasto-viscoplastic (TEV) crystal plasticity constitutive formulation is developed and implemented in the well-known Marciniak-Kuczynski (1967) analysis to predict the limit strains of AA5754 and AA3003 for various strain paths at elevated temperatures. The model takes into account the temperature dependence of the single crystal elastic coefficients, single slip hardening parameters, thermal softening, slip rate sensitivity, and the total deformation. Temperature dependent single slip hardening parameters are determined from uniaxial tension simulations at room and elevated temperatures. The new model employs the so-called Taylor homogenization scheme and is able to accurately predict the experimental forming limit diagrams (FLDs) without the need for further curve fitting. The effects of elastic constants and thermal softening on FLD predictions are discussed, and a new expression to represent the temperature dependence of the initial imperfection (for the M-K analysis) is developed to enable the model to successfully predict the FLDs of AA5754 and AA3003 for any temperature in the warm forming regime prior to recrystallization.

13th U.S. National Congress on Computational Mechanics
July 27-30, 2015, San Diego, California, USA

Title: Verification and Validation Studies of Ordinary Peridynamic Solid Models

Author(s): John Mitchell, *Sandia Nat'l. Lab.*.

SAND2015-0899 A ---------- Ordinary-state-based peridynamics models [Silling, 2007] are a generalization of bond-based peridynamic models; the force state at a point depends upon the collective deformation of the family of points defined by the length scale 'horizon'. Furthermore, ordinary state-based peridynamic models generally do not exhibit numerical instabilities that arise when using a correspondence approach, and they remove the Poisson ratio = .25 limitation of bond-based models. In recent years, the linear peridynamic solid model LPS [Silling, 2007] has been extended to include viscoelastic and plastic deformations [Mitchell, 2011]. In this talk, I will present work towards verifying and validating ordinary-state-based models in the absence of fracture. Keywords -------- peridynamics, nonlocal, ordinary-state-based, verification, validation References ---------- * Silling, S.A. and Epton, M. and Weckner, O. and Xu, J. and Askari, E., Peridynamic States and Constitutive Modeling, Journal of Elasticity, pages 151--184, Volume = 88, Year = 2007. * Mitchell, J.A., A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics, Sandia Report SAND2011-3166, Sandia National Laboratories, Albuquerque, NM, May, 2011. * Mitchell, J.A., A non-local, ordinary-state-based viscoelasticity model for peridynamics. Sandia Report SAND2011-8064, Sandia National Laboratories, Albuquerque, NM, May, 2011. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

13th U.S. National Congress on Computational Mechanics
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Title: VoroCrust Geometry: 3D Polyhedral Meshing with True Voronoi Cells Conforming to Prescribed Surface Points

Author(s): Ahmed Mahmoud, *Alexandria U.*; Ahmad Rushdi, Chandrajit Bajaj, *UT Austin*; Scott Mitchell, Mohamed Ebeida, *Sandia Nat'l. Lab.*; John Owens, *UC Davis*.

We introduce VoroCrust for creating polyhedral meshes of 3D solids enclosed by 2D surfaces. VoroCrust is the first algorithm for 3D Voronoi meshes that naturally *conform* to prescribed surface points. Conformality is distinguished from the usual *clipping* of Voronoi cells by the surface, which always results in extra surface vertices beyond the original samples, and may result in non-planar, non-convex, or even non-star-shaped cells. VoroCrust creates cell seeds such that the original points on the surface manifold are vertices of the 3D cells, and the only surface vertices. This avoids shrinkage and other changes. All cells are true Voronoi cells; the surface does not restrict or constrain the Voronoi cells, rather the cells are geometrically placed to reconstruct the surface, by the cell facets separating inside and outside seeds. These facets are well-shaped and usually triangles. Mesh polyhedra enjoy all the nice properties of Voronoi cells, such as being convex with planar facets. Cell aspect ratios and dihedral angles are bounded. We have not yet addressed the issues of small edges, sharp edge angles, and small area faces, which may be important for some types of simulations. In contrast to the well-known “power crust” surface reconstruction algorithm, VoroCrust fills the volume with tunable 3D cells with good shape, and its 2D manifold reconstruction is from an *unweighted* Voronoi diagram. The VoroCrust algorithm starts with sample points capturing small and sharp surface features, and are dense compared to the local thinness and curvature. We can create these by Maximal Poisson-disk Sampling (MPS), or the points may be given as input. In either case we create a sphere around each sample. Some triples of overlapping spheres define a pair of intersection points, mirrored on each side of the manifold. Pairs outside all other spheres are analogous to weighted triangulation circumcenters, lifted above (and sunk below) the manifold according to its weighted distance. These are Voronoi seeds. We add well-spaced seeds in the far interior; these may be chosen to create a hex-dominant mesh. We generate the 3D Voronoi tessellation of all these seeds. The manifold is reconstructed by the Voronoi facets separating the inside and outside cells, the lifted and sunk seed pairs. This talk describes the geometry of VoroCrust, the primal-dual-dual-primal dance and the power center lifting. Mohamed Ebeida’s talk in session MS711, “Polygonal and Polyhedral Discretizations in Computational Mechanics,” describes the engineering aspects of VoroCrust.

13th U.S. National Congress on Computational Mechanics
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Title: Optimal Nanostructures for Li-Ion Battery Anode Applications

Author(s): Sarah Mitchell, Michael Ortiz, *California Inst. Tech.*.

The lithium-ion battery is one of the most widely used commercial batteries, powering electric vehicles and portable electronic devices such laptops, smart phones and cameras. There has been significant interest in developing an anode structure in a lithium-ion battery that exhibits superior performance over a traditional graphite anode in terms of energy density, cyclability and mechanical robustness. An ideal anode material under consideration is silicon, which has a theoretical specific capacity ten times higher than graphite. However, a 300% volume expansion and contraction of the silicon anode occurs during lithium insertion and extraction. This has significant detrimental effects such as pulverization of the active alloy particles and mechanical fracture that cause a reduction in specific capacity with cycling, resulting in a very limited life cycle. One possible method of overcoming the volume expansion during lithiation cycles is utilizing topology optimization methods to determine an optimum periodic composite anode truss structure on the micro to nano-meter range, consisting of a conductive copper core and a silicon outer layer. A density-based material distribution method employing the modified solid isotropic material with penalization (SIMP) procedure is used in conjunction with iteratively performing finite element analysis, sensitivity analysis, filtering and optimization steps to determine the optimum distribution of material within a periodic base cell subject to a given set of loading and boundary conditions. Design requirements of minimum volume expansion, high energy density and periodicity dictate the need for topology optimization with multiobjectives. A weighted average method is used to evaluate a Pareto optimum. Results show the optimal structure is dependent on the value of the Pareto weights, therefore a trade off in competing design objectives is necessary. Pareto front, convergence and mesh independence studies are conducted to validate results.

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Title: Non-Linear Coupling of the Drift-Diffusion-Poisson and Stokes Systems for Nanopore Simulations

Author(s): Gregor Mitscha-Eibl, Andreas Buttinger-Kreuzhuber, Gerhard Tulzer, *TU Vienna*; Clemens Heitzinger, *TU Vienna; Arizona State U.*.

Introduction Nanopore sensors with radii in the nanometer range have been manufactured based on alpha-hemolysin, DNA-origami structures, and solid-state membranes in recent years. By applying an electric field to the electrolyte and measuring the ionic current as target molecules translocate the pore, nanopore devices can be used as high-precision sensors. Applications include single-molecule detection and next-generation DNA sequencing. Predictive mathematical models and simulations are needed for the rational design of nanopore devices. The model equations Our nonlinear steady-state multi-physics model consists of the drift-diffusion-Poisson system for the electric potential and ion concentrations, coupled with the Stokes system modeling the water flow. A biomolecule is placed inside the pore. Even in reduced, i.e., axisymmetric 2D models, the large number of scalar unknowns – 6 in the standard case of two different ion species –, the nonlinearity, as well as multiscale features of the solutions such as strong boundary layers induced by surface charges pose a significant challenge to numerical simulation. The numerical method Since this particular set of equations has so far hardly been addressed in the numerical literature, one of the first objectives was to find a suitable method to resolve the nonlinearity. An advantageous choice was found to be a hybrid strategy of decoupling the Stokes part by a fixed-point iteration and solving the remaining drift-diffusion-Poisson system by a Newton method. This greatly reduces the computational effort compared to a straightforward application of the Newton method to the whole system. An additional difficulty is introduced when calculating the forces on a translocating molecule. This force involves the gradient of the flow velocity at the molecule surface and is therefore highly sensitive to inaccuracies of the Stokes approximation. To reach the desired accuracy in acceptable time, high-order discretizations as well as a strongly refined mesh near the surface seem to be mandatory, which makes our problem an interesting case study for goal-oriented adaptive error control. Our finite-element implementation is based on the FEniCS package. Using the above approach, the run time for the coupled system in 2D is only several minutes. Conclusions We have developed a fast numerical approach for the drift-diffusion-Stokes-Poisson system to calculate all fluxes through nanopores and the forces acting on target molecules. Very good agreement between measurements and simulations has been found.

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Title: Shape Optimization of a Corrugated Airfoil and Planform Optimization of a Finite Wing

Author(s): Varun Bhatt, Sambhav Jain, Sanjay Mittal, *Indian Inst. Tech., Kanpur*.

Key Words: corrugations, shape optimization, planform The effect of corrugations on the aerodynamic performance of a Mueller C4 airfoil, placed at a 5° angle of attack, is investigated via 2D computations. The flow is governed by the incompressible Navier Stokes equations. A stabilized finite element method is employed. The Reynolds number based on the chord length of the airfoil and free stream speed of the flow is 10,000. Computations are carried out for different location and number of corrugations, while holding their height (h=1.5%c) fixed. The effect of these corrugations on the aerodynamic performance of the airfoil is investigated. The aerodynamic efficiency of the airfoil with four corrugations is 21% higher compared to Mueller C4 airfoil. Further, Shape optimization of the Mueller C4 airfoil is carried out using various objective functions and optimization strategies. The different strategies used for optimization are referred to as PCOT (Preserve camber, optimize thickness), PTOC (Preserve thickness, optimize camber) and NCCT (No constraint on camber or thickness). The objective functions are maximization of lift, minimization of drag and maximization of aerodynamic efficiency. The optimal shape obtained via the PTOC strategy performs the best, leading to 50% increase in lift coefficient and 23% increase in aerodynamic efficiency compared to the Mueller C4 airfoil. Planform optimization is performed for a finite wing with rounded wingtip. The objective is to find an optimal planform with maximum aerodynamic efficiency. The 3D computations are done for a finite wing at Re = 1000 and angle of attack 4o. The wing semi-span is kept fixed to 5 units. The cross-section of the wing is NACA 0012 throughout. In order to obtain optimal planform, chords at different spanwise stations are allowed to move along the streamwise direction and chord-lengths are allowed to vary. Two different strategy referred to as symmetrical constrained optimization and unsymmetrical constrained optimization are considered. Different planforms i.e. rectangular planform and elliptical planforms are considered for the optimization as initial guesses. The optimal planform obtained via the unsymmetrical constrained optimization for elliptical planform performs the best, leading to 19% increase in aerodynamic efficiency compared to the elliptical planform. REFERENCES [1] Srinath D., Mittal S., 2010. An adjoint method for shape optimization in unsteady viscous flows, Journal of Computational Physics, 229, 1994-2008. [2] Srinath D., Mittal S., 2007, A stabilized finite element method for shape optimization in low Reynolds number flows, International Journal for Numerical Methods in Fluids, 54, 1451-1471.

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Title: Dislocation Dynamics Simulation of Transition of Dislocation-Precipitate Interaction Mechanism

Author(s): Masaki Miyagi, Akiyuki Takahashi, *Tokyo U. Science*.

Precipitation strengthening is a technique for designing alloys with desired strength. In the precipitation strengthening, nano-sized precipitates are distributed, and gives significant influence to dislocation motion. As the result, the material strength, such as yield stress and flow stress, can be improved. In the interaction between a dislocation and a precipitate, the dislocation cuts the precipitate, and goes over the precipitate (cutting mechanism). In addition, if the size of precipitate is large enough, the mechanism might be changed to the Orowan mechanism, where dislocations cannot cut the precipitate, and go around the precipitate. Finally the dislocation leaves a dislocation loop around the precipitate. However, the detailed information on the transition of the dislocation-precipitate interaction mechanism has not been clarified yet, although the information must be significant in designing high-strength alloys using the precipitation strengthening. In this study, we use the dislocation dynamics method to investigate the transition of the dislocation-precipitate interaction mechanism. In the simulation, we simply simulate the behavior of one dislocation, and interaction between the dislocation and a precipitate. Then, the critical resolved shear stress (CRSS), which is the shear stress necessary for dislocations to go over precipitates, is calculated. The influence of the diameter of precipitate and interspacing between neighboring precipitate on the transition of dislocation-precipitate interaction mechanism is investigated. Then, the calculated CRSS is compared to analytical solutions of CRSS. It could be found that the transition occurs continuously in terms of CRSS, and the influence of dislocation bending is significant in determining the CRSS of cutting mechanism.

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Title: RANS and Detached-Eddy Simulations of Wingtip Vortices Around NACA0012 Wing by a High-Order Accurate Flux Reconstruction Approach

Author(s): Koji Miyaji, *Yokohama Nat'l. U.*.

Unsteady flows around a NACA0012-wingtip are numerically simulated toward identifying the source of an aerodynamic noise of high-lift devices. The flow Mach number is 0.175, the angle of attack is 12 degrees and Reynolds number based on the chord length is 1.8 million[1]. A high-order accurate flux reconstruction (FR) approach[2] is developed to simulate the Reynolds-averaged Navier-Stokes equations and the k-w two-equation turbulence model. We specifically used Legendre-Gauss solution points and Radau polynomial as the flux correction function, which is a counterpart of the discontinuous Galerkin (DG) method in the framework of the FR. To author's knowledge, this is the first trial to use the k-w model in the FR flow simulations. The same numerical methodology employed in DG to include the k-w model[3] was found effective in the FR as well. The model has been further extended to the detached-eddy simulation by a slight modification for the switching term. The effects of grid resolutions, the order of spatial accuracies and the RANS/DES mode have been investigated by comparing with time-averaged and unsteady pressure measurement. We have calculated so far 2nd-order accuracy with 0.5 M and 1.5 M degrees-of-freedom (DOFs) and 3rd-order accuracy with 1.5 M DOFs. Flow features characterized by the two wingtip vortices, one emanating from the lower surface and the other emanating from the wingtip surface, are better resolved by the 3rd-order case. The suction peaks represented by the pressure distributions quantitatively show the improvement against the 2nd-order FR cases and the finite-volume simulation results in our previous study. In the preliminary study of DES, the suction peaks further compare well with the experiment, possibly due to the suppression of excessive eddy viscosities. The simulations are ongoing. We have developed an implicit LU-SGS method with 2nd-order time accuracy and we will continue time-accurate simulations to evaluate unsteady pressure fluctuations on the wing. The magnitude and frequencies of the sound pressure level are to be extracted from the simulation results. [1] Imamura, T. , Enomoto, S., and Yamamoto, K., "Noise Generation Around NACA0012 Wingtip Using Large-Eddy-Simulation," 25th International Congress of the Aeronautical Sciences, ICAS 2006. [2] Huynh, H. T., "A Flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods," AIAA paper 2007-4079. [3] Bassi, F., Crivellini, A., Rebay, S., and Savini, M., "Discontinuous Galerkin Solution of the Rynolds-averaged Navier-Stokes and k-w turbulence model equations," Computer and Fluids 34 (2005) 507-540.

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Title: Three-Dimensional Crack Nucleation, Growth and Coalescence Using the Thick Level Set Approach to Fracture

Author(s): Nicolas Moes, Alexis Salzman, Nicolas Chevaugeon, *EC-Nantes*.

The thick level set (TLS) model is a unified theoretical model able to model nucleation, growth and coalescence of cracks. It is based on a non-local model for damage. Its originality with respect to existing other non-local damage model (integral, second order, phase-field, …) is twofold. First, the boundary of the fully damage area (crack) is explicitly given by a level set. The introduction of a discontinuous kinematic is thus made easy in particular with the extended finite element method (X-FEM). The crack placement adjusts exactly to damage growth. This avoids drawbacks of ad hoc crack placement in damage zone, that is: convergence issue of the global solve if the crack is placed too late and abrupt loss or energy if the crack is placed too quickly. In the latter case, a remedy is to introduce a cohesive crack but this requires yet another model on top of the damage model. The second originality of the TLS is that non-local damage is restricted to a narrow band around the crack. The extra cost to deal with non-locality is thus small. Both originalities stem from the fact that the non-locality of damage is formulated by an Eikonal constraint and not a Laplacian constraint. Three-dimensional examples will demonstrate the capability of the TLS to model crack initiation, growth and coalescence. References [1] Moës, N., Stolz, C., Bernard, P.-E., & Chevaugeon, N. (2011). A level set based model for damage growth : the thick level set approach. International Journal For Numerical Methods in Engineering, 86, 358–380. [2] Bernard, P.-E., Moës, N., & Chevaugeon, N. (2012). Damage growth modeling using the Thick Level Set (TLS) approach: Efficient discretization for quasi-static loadings. Computer Methods in Applied Mechanics and Engineering, 233-236, 11–27. [3] Stolz, C., & Moës, N. (2012). A new model of damage : a moving thick layer approach. International Journal of Fracture, 174(1), 49–60.

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Title: Three-Dimensional Simulator for Pressurized Cracks

Author(s): Dmitry Nikolskiy, Sofia Mogilevskaya, *U. Minnesota*.

Computational modeling of hydraulic fracturing process involves the coupling of several processes [1]. One of them is the process of mechanical deformation induced by the fluid pressure. This paper reports new developments on computational modeling of three-dimensional problems of pressurized cracks of arbitrary shapes. The approach employs planar triangular boundary elements and is based on the integral representations written in a local coordinate system of an element. In-plane components of the fields involved in the representations are separated and arranged in certain complex combinations. The unknown functions involved in the representations are approximated by quadratic polynomials. An efficient technique is developed for analytical evaluation of the boundary integrals [2]. Several illustrative numerical examples involving a single (penny-shaped) crack and multiple (semi-cylindrical) cracks are presented. References 1. Adachi J., Siebrits E., Peirce A., Desroches J. Computer simulation of hydraulic fractures. International Journal of Rock Mechanics and Mining Sciences 2007; 44: 739-757 2. Mogilevskaya S.G., Nikolskiy D.V. The use of complex integral representations for analytical evaluation of three-dimensional BEM integrals. Potential and Elasticity problems. The Quarterly Journal of Mechanics and Applied Mathematics 2014; 67: 505-523

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Title: Lattice Simulation for Evaluating Fracture Properties of Brick-Mortar Interfaces Using Four-Point Bending Tests

Author(s): Amir H. Mohammadipour, Reza Mousavi, Kaspar Willam, *U. Houston*.

This study focuses on lattice-based fracture simulations to characterize progressive debonding of brick-mortar interfaces in unreinforced masonry composites using a notched four point bending benchmark problem. A 2-D lattice formulation was implemented to evaluate interface fracture properties of a composite notched beam made of clay brick substrate bonded to a mortar overlay layer by a single layer of strut interfaces. Discretization of the continuum brick and mortar domains are based on Voronoi tessellation. Different strength failure criteria are assigned to brick, mortar, and interface strength material properties that are mapped on top of the mechanical model of the lattice according to their geometric locations. Energy release and crack surface displacement (CSD) methods were considered to evaluate the fracture properties of interfacial crack growth. The energy release rate of the interface was obtained by the change in the global stiffness matrix of the lattice model before and after of interfacial strut removal. This energy release rate was inserted into the Irwin type fracture relationship for plane strain to calculate the modulus of complex stress intensity factor which is independent of the distance from the crack tip. In the CSD method, the relative plane strain displacements of interfacial crack surfaces in the form of opening mode I and slip mode II were evaluated by the lattice model behind the crack tip at an appropriate distance. These relative displacements may be expressed in the complex plane representing the interface crack in terms of a complex intensity factor leading to the determination of stress intensity factors for mode I and mode II along with the phase angle of loading. In summary, the computational lattice model is capable of evaluating the fracture toughness of brick-mortar interface along with other fracture properties from basic strength properties of lattice struts, which are removed by erosion upon failure. This information is employed to upscale the lattice fracture arguments onto the meso-scale to quantify the fracture energy formulation of traction-separation cohesive zone models in the context of continuum finite element simulations of heterogeneous media such as masonry.

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Title: A Global Meta-Model for Multidisciplinary Design Optimization

Author(s): Yaghob Gholipour, Parviz Mohammedzadeh, *U. Tehran*.

Most industrial engineering design problems are multidisciplinary in nature (e.g. aerospace and automotive). Multidisciplinary design optimization (MDO) has become an effective method for solving these industrial design problems. Collaborative optimization (CO) is one of the main MDO approaches for solving multidisciplinary design problems. The main difficulties associated with MDO are often characterized by interdisciplinary couplings, high computational cost of an analysis in individual disciplines and a large number of design variables and constraints. These issues result in very high overall computational cost limiting applications of MDO to complex industrial design problems. To address these issues a combination of global meta-model using moving least squares (MLSM) and the trust region strategy is introduced. The use of meta-models or approximations in design optimization in general and MDO in particular has become popular for reducing the computational cost and filtering out the numerical noise of high fidelity models in the optimization process. In addition, it provides a means for rapid design space exploration and more importantly, visualization of the design search space. The basic approach is to replace computationally expensive high fidelity model by an approximate one, which is computationally very efficient model. In this paper, a global meta-model is used to identify the feasible and infeasible regions and the trust region strategy is used for a detailed search of the feasible region. The technique is demonstrated on a test problem and the effectiveness of the method for modeling and system level collaborative optimization using high fidelity models is studied. The results show that meta-model based on MLSM provide a high degree of accuracy whilst achieving a considerable reduction in computational cost. Keyword: multidisciplinary design optimization, meta-model, moving least squares method, collaborative optimization and trust region strategy

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Title: Energetics and Kinetics of the Vacancy Phase-Field-Crystal Model

Author(s): David Montiel, Katsuyo Thornton, *U. Michigan*.

Over the last decade, the Phase Field Crystal (PFC) model has proven to be a powerful computational tool for studying materials phenomena at atomic length scales and diffusive time scales. The model serves to bridge the gap between molecular dynamics (MD) and traditional (coarse grained) phase field models. It has been applied to study, for example, liquid-solid transitions, grain-boundary dynamics, motion of dislocations, and glass formation. After an overview of our work in the field, we present a study on the stability of individual vacancies in the Vacancy PFC (VPFC) model. By fitting data from numerical simulations, we obtain an equation of state for the equilibrium vacancy concentration in an otherwise perfect crystal. We show how the equilibrium vacancy concentration depends on the system's average density and on the undercooling parameter. We also obtain a phase diagram for the system consisting of the 'perfect crystal' and 'vacancy' phases. The phase diagram is compared with those obtained from two theoretical models. In the first theoretical model, the density profile is described by the one-mode approximation. In the second model, we use non-overlapping Gaussians to describe the atomic peaks. We show that the latter provides a better approximation. Finally, we study the effect of the adjustable parameters in the VPFC dynamics on the stability and diffusion of individual vacancies.

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Title: Molecular Dynamics Studies of the Effect of Initial Chain Orientation on the Shape Recovery Behavior of Polystyrene

Author(s): Junghwan Moon, Joonmyung Choi, Maenghyo Cho, *Seoul Nat'l. U.*.

Shape memory polymers (SMPs) can change their shapes and mechanical properties in response to the external stimuli such as heat, electric/magnetic field or even light irradiation.Especially, pre-strained polystyrene (PS) sheets (e.g. Shrinky-Dinks) with simple two dimensional patterns show self-folding behavior by infrared (IR) light heating[1].Actuation of PS sheets by light has distinct advantages like the remote and wireless control and realization of complex deformation with simple manner. Here, molecular dynamics (MD) simulation isexecuted to examine a relationbetweenthe initial orientational order of polymer chains and shape recovery behavior of PS. Amorphous atactic PS unit cells with two different molecular weights (20,000 and 40,000 g/mol) are prepared.For each constructed model, shape memory cycle isdescribed by stepwise manner: heating up above glass transition temperature (Tg), biaxial tensile deformation, cooling down below Tg, stress relaxation, and re-heating with the heating rate of 5 K/ns.The cells with three different oriented state (= 30, 60, 100%) are considered to compare the shape recovery behaviors. During the re-heating process, shrinkage of unit cell in the initially oriented direction and expansion in the normal direction are simultaneously observed. The initiation temperature of shrinkageis higher and the phasetransitionrange is wider with more oriented PS. Also, the collapse of initial orientation occurs and the unit cells become isotropic stateduring thermal shrinkage. The recovery rateof transition to the isotropic state is slower with more initial chain orientation. The shape recovery of unit cell is fully completed with the initial strain of 30%. However, the residual strain remains for the cases with 60% and 100% strain even after the orientations of internal polymer chains are collapsed. In the oriented state, tensile modulus along the oriented in-plane direction is higher than that of out-of-plane direction. This anisotropy is diminished during the re-heating simulation. These results are helpful to understand and systematically design the macroscopic self-folding behaviorsinfluenced by the microscopic initial orientation of PS. [1] Y. Liu, J. K. Boyles, J. Genzer, and M. D. Dickey, Soft Matter 8, 1764-1769 (2012).

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Title: Fluid-Structure Interaction with Finite Volume Method in Both Domains

Author(s): M. R. Moosavi, *S. Dakota State U.*.

This work is concerned with the modeling of the interaction of Newtonian and non-Newtonian fluid flow with flexible solid structure. The fluid flow considered is governed by the incompressible Navier–Stokes equations. Both Newtonian and non-Newtonian flows can be solved by the fluid solver. The structure is represented by means of an appropriate finite volume formulation. In the interface of two domains, the pressure and shear traction from the fluid part are interpolated to the solid part as applied load on the solid domain and the solid displacement is interpolated to the fluid part as the new boundary conditions in the fluid domain. The meshes are moved by using the Laplacian method in each time step. The solid solution is relaxed by applying the adaptive Aitken relaxation technique. The method has been verified in the fluid, solid, and coupled domains separately. The solver of the fluid domain can produced good results in a lid-driven cavity benchmark with Newtonian and Power-law flow. In solid domain, the solver can present good results for a plate with a central hole under traction. A lid-driven cavity with flexible bottom wall is considered as a benchmark for the coupling domains. The results show a good performance of the method to solve coupled problems in fluid-structure interaction. Finally, numerical results of a real extrusion die with flexible top wall are presented. The results indicate the procedure has effectively practical capability of simulation of different fluid-structure interaction problems. References: 1. C. Förster, W.A. Wall, E. Ramm, Artificial added mass instabilities in sequential staggered coupling of nonlinear structures and incompressible viscous flows, J. Comput. Methods Appl. Mech. Engng. 196 (2007) 1278-1293. 2. K.J. Bathe, H. Zhang, A mesh adaptivity procedure for CFD and fluid-structure interactions, Comput. Struct. 87 (2009) 604–617.

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Title: Topology Optimization Method Applied to the Design of a Rotating Piezo-Structure Subjected to Active Control Law

Author(s): Mariana Moretti, Emílio Silva, *U. São Paulo*; Wilfredo Rubio, *Nat'l. U. Colombia*.

Robotic arms for pick and place of lightweight materials are broadly employed in industry nowadays. A simple model of such a robotic arm consists of a beam like structure attached to a motor shaft that works under high angular velocity and low tip loads. This kind of structure may present high amplitude of residual vibrations, which is not interesting for high precision applications such as the one proposed in this work. Previous topology optimization approaches to similar problems have succeeded in attenuating the residual vibrations by maximizing the strain energy by kinetic energy ratio by applying the equivalent static load method to circumvent the problem of performing the sensitivity analysis in dynamic response optimization scheme. However, it is also desirable that the stabilization time occurs before the motion track path reaches its end at a set up angular velocity. Leveraging the reachability of such a transient response, the present work applies an active control law to the structure in order to obtain an optimal topology for specific transient response parameters. The aforementioned control law will rely on piezoelectric ceramics. As they convert mechanical displacements to electrical charges and vice-versa, two of these piezoceramics are coupled to the structure, one for sensing purpose and the other one for actuating purpose. The piezoceramics have fixed positions within the domain while the metallic structure layout is designed by using Topology Optimization Method (TOM). Two metallic materials composes the designed domain as TOM is implemented based on the SIMP material model for two types of design variables, taking advantage of a multi-material concept including the Functionally Graded Material formulation. The current amplifier definition is applied to convert the sensor output into a voltage input on the actuator by means of a specified feedback gain. Therefore, the general problem is stated as a minimization of the strain energy restricted to a maximum material volume and the dynamic equilibrium equation, which accounts with a gain velocity feedback law. The sensitivity analysis is calculated by means of the adjoint method while its discrete approximation is evaluated with a direct time integration method after the continuous function differentiation is taken, an approach denominated differentiate-than-discretize. Examples are restricted to two-dimensional models in which the influence of feedback control gain is discussed over the output response attenuation and stabilization time.

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Title: Analysis-Suitable Adaptive T-Mesh Refinement with Linear Complexity

Author(s): Philipp Morgenstern, Daniel Peterseim, *U. Bonn*.

T-splines have been introduced as a free-form geometric technology and are one of the most promising features in Isogeometric Analysis. Since T-splines can be locally refined, they potentially link the powerful geometric concept of Non-Uniform Rational B-Splines (NURBS) to meshes with T-junctions and hence the well-established framework of adaptive mesh refinement. However, it was shown that T-meshes can induce linear dependent T-spline blending functions. This prohibits the use of T-splines as a basis for analytical purposes such as solving a partial differential equation. This insight motivated the research on T-meshes that guarantee the linear independence of the corresponding T-spline blending functions, referred to as analysis-suitable T-meshes. In this talk, we present a new refinement algorithm which provides (1) the preservation of analysis-suitability and nestedness of the generated T-spline spaces, (2) a bounded cardinality of the overlay (which is the coarsest common refinement of two meshes), (3) linear computational complexity of the refinement procedure in the sense that there is a constant bound, depending only on the polynomial degree of the T-spline blending functions, on the ratio between the number of generated elements in the fine mesh and the number of marked elements in all refinement steps. For reference, see http://arxiv.org/pdf/1407.6175v4.pdf .

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Title: Stochastic Inadequacy Operators: A Case Study in Methane Combustion

Author(s): Rebecca Morrison, Robert D. Moser, Todd A. Oliver, *UT Austin*.

We investigate model inadequacy for a reaction mechanism model in methane combustion. In a typical reaction involving hydrocarbons, the complete mechanism is either not well-understood, or too complex to effectively use as part of a larger combustion problem, necessitating a reduced model. To account for the discrepancy between the high-fidelity model and its reduced version, we propose an additive, linear, probabilistic formulation. This representation is encoded in a random matrix, whose entries are calibrated using a high-dimensional hierarchical Bayesian scheme. In particular, this formulation is designed to respect certain physical constraints, but also be flexible enough to apply to multiple reactions.

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Title: Highly Scalable Framework for Fully Coupled Multi-Scale Simulation of Failure in Heterogeneous Layers

Author(s): Matthew Mosby, Karel Matous, *U. Notre Dame*.

Multiscale phenomena are ubiquitous in engineering science and are increasingly important in design of structures and materials. For instance, current structural designs frequently make use of adhesive joints in favor of more traditional fastening techniques for ease of manufacturing and reduction of stress concentrations. Most modern adhesives are highly heterogeneous, containing a wide range of sizes, shapes, and material properties of reinforcing constituents. Unfortunately, these adhesive joints and/or layers are often the weak link in the load bearing capacity of bonded structures. Understanding how changes in the adhesive layer morphology effect the overall mechanical response of bonded systems is important for design and safety assessment. Direct Numerical Modeling (DNM), which captures all relevant physical length scales in a single large simulation, is one method for accurately predicting the multiscale failure response. However, the computational domains required to resolve physical features from the scale of the bonded assembly down to the failure zone thickness within the adhesive layer are extremely large and often too computationally expensive to solve, even for modern supercomputers. Therefore, we have developed a hierarchically parallel scale-bridging solver based on the theory of Computational Homogenization (CH) for thin layers to simulate multiscale failure of adhesively bonded systems in the 3D finite strain setting. The CH theory assumes a separation of scales, and locally attaches a Representative Unit Cell (RUC) of the adhesive layer to each material point on the macroscopic interface. The macroscale and microscale response is linked through the variational energy equivalence (Hill's lemma) for interfaces. Thus, the macroscopic traction-separation response is computationally derived from the microscale, where material behavior of the individual constituents is better understood. In this presentation, we detail the computational implementation of the hierarchically parallel solver and demonstrate its high scalability to over 65 thousand computing cores. We use this solver to compute the multiscale failure response of O(cm) bonded mechanical devices with up to O(10 nm) numerical resolution using Billions of finite elements. We show that such large simulations are possible using a modest number of computing cores, while solutions may be obtained faster using more resources. The ability to efficiently compute such detailed simulations is important for uncertainty quantification and development of materials by design.

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Title: Seeing the Bigger Picture: Comparing One-Dimensional and Multi-Dimensional Interpolation Algorithms in Remap

Author(s): Stewart Mosso, *Sandia Nat'l. Lab.*; Richard Kramer, .

The traditional method of remapping conserved quantities in Volume of Fluid simulations is to employ alternating direction, one-dimensional remaps. These algorithms typically use a one-dimensional interpolation algorithm such as van Leer's MUSCL algorithm. Recently the authors developed a multi-dimensional, conservative, third-order algorithm based upon van Leer's. A matter of conjecture has been how much dissipation the one-dimensional MUSCL introduces due to its limited, one-dimensional view of the fluxing neighborhood. On the other hand, the multi-dimensional algorithm uses a larger stencil in its interpolation which through its monotonicity constraints will introduce dissipation as well. This talk will compare the accuracy and dissipation for both one-dimensional and multi-dimensional algorithms using single material verification problems.

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Title: The Alternating Schwarz Method for Concurrent Multi-Scale in Finite Deformation Solid Mechanics

Author(s): Alejandro Mota, Irina Tezaur, *Sandia Nat'l. Lab.*.

Multiscale methods are becoming prevalent in the analysis of solid mechanics problems in which it is necessary to bridge time or length scales to account for fast or small processes. These methods are of most relevance in the simulation of damage, failure or crack initiation where the information needs to flow to and from the different scales to capture these phenomena reliably. Here, we propose a novel multiscale approach in which the Alternating Schwarz Method is used as a means to couple different scales concurrently. The Alternating Schwarz Method is a well-established technique for the solution of elliptic PDEs by means of domain decomposition. Unlike traditional multiscale coupling approaches, the Schwarz method avoids the use of Lagrange multipliers or gradients. In this talk, we discuss the implementation of the method in the open-source Albany finite element platform developed at Sandia National Laboratories and demonstrate the effectiveness of the method for concurrent coupling in finite deformation solid mechanics in quasi-statics. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Adaptive Spectral Finite-Element Based Computational Methods for Large-Scale Electronic Structure Calculations Using Kohn-Sham Density Functional Theory

Author(s): Phani Motamarri, Vikram Gavini, *U. Michigan-Ann Arbor*.

Quantum-mechanically informed calculations based on Kohn-Sham density functional theory (DFT) have provided many important insights into wide range of materials properties over the past decade. However, large-scale DFT calculations are computationally very demanding and hence have been primarily associated with either plane-wave basis or atomic-orbital basis sets which severely restrict the type of boundary conditions or the geometry associated with materials systems studied. Among real-space techniques for DFT, finite-element (FE) discretization of Kohn-Sham density functional theory (DFT) is versatile and is amenable for unstructured coarse-graining, allows for consideration of complex geometries and boundary conditions, and is scalable on parallel computing platforms. However, the apparent shortcomings in the use of FE discretization for DFT such as, the requirement of very large number of basis functions coupled with cubic computational complexity of DFT and the non-orthogonality of the basis functions have made it less attractive for large scale calculations, severely limiting the size of materials systems to few hundreds of electrons. This work tries to address these shortcomings by developing a new computationally efficient and robust finite-element based parallel algorithms (DFT-FE) to enable large-scale DFT calculations. The proposed DFT-FE enabled for the first time a simulation of the electronic structure of materials system as large as 7000 atoms (14000 valence electrons) using finite-element basis. The key ideas in the development of DFT-FE include i) a real-space adaptive higher-order spectral finite-element framework which can handle all-electron and pseudopotential calculations with complex boundary conditions on a single footing, (ii) a subspace projection method to reduce the computational complexity of DFT calculations while treating metallic and insulating materials in a single finite-element framework and (iii) a configurational force approach to efficiently compute forces on atoms in order to find the most stable geometry. The numerical investigations conducted with DFT-FE on representative benchmark examples show that computational efficiency of finite-element basis is competing with commercial codes using plane-wave basis (smooth pseudopotential calculations), and compares well with atomic-orbital basis (all-electron calculations with singular potentials) and show excellent parallel scalability. Furthermore, the benchmark studies involving pseudopotential calculations on metallic aluminum nano-clusters (up to 3500 atoms) and on insulating alkane chains (up to 7000 atoms) as well as all-electron calculations on semi-conducting silicon nano-clusters (up to 4000 electrons), reveal that the proposed subspace projection algorithm exhibits subquadratic-scaling behavior with system size along with accuracies commensurate with chemical accuracy. Signifcant computational savings have been realized with 10 fold speedups observed for the largest systems with respect to previous reference calculations

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Title: Mechanical Basis of Seashell Morphology

Author(s): Derek Moulton, Alain Goriely, *U. Oxford*; Régis Chirat, *U. Lyon* .

Seashells have intrigued scientists and mathematicians alike for centuries. Over the past several hundred years paleontologists have amassed a huge body of observations on shell form and its evolutionary variation and diversification. However, though the patterns in shells have been well documented, the formation of those patterns has only been explained in functional terms, while the developmental mechanisms underlying shell morphogenesis have remained largely elusive. I will present work on a mechanical basis for shell morphogenesis, using models based on the geometry and fundamental principles of the growth process. We first develop a mathematical framework to describe the accretionary growth of shells, based on local shell geometry and utilising differential geometry of curves[1]. We then turn to the nearly ubiquitous presence of shell ornamentation such as spines and ribs. Working within the framework of elasticity, we demonstrate how the mechanical interactions of the accreting tissue of the mollusc and the rigid shell to which it adheres provides a mechanism for the formation of shell ornamentation, and indeed seems to account naturally for the great diversity of ornamentation patterns[2,3]. [1] Moulton, D. E., & Goriely, A. (2014). Surface growth kinematics via local curve evolution. Journal of Mathematical Biology, 68(1-2), 81–108. [2] Chirat, R., Moulton, D. E., & Goriely, A. (2013). Mechanical basis of morphogenesis and convergent evolution of spiny seashells. PNAS, 110(15), 6015–6020. [3] Moulton, D. E., Goriely, A., & Chirat, R. (2015). The morpho-mechanical basis of ammonite form. Journal of Theoretical Biology, 364(C), 220–230.

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Title: Finite Element Simulations of Dynamic Shear Localization in Elasto-Viscoplastic Solids Under Adiabatic Conditions

Author(s): Hashem Mourad, *Los Alamos Nat'l. Lab.*; Curt Bronkhorst, *Los Alamos Nat'l Lab.*.

Failure of metallic materials is often preceded by the formation of narrow bands of localized plastic strain. Here, a sub-grid computational formulation, implemented in an explicit Lagrangian framework, is used to study the formation of such shear bands under high-rate dynamic loading. The sub-grid technique allows a shear band to be embedded within a computational element, thereby alleviating mesh sensitivity and obviating the need to resolve the small-scale process zone. It also allows the use of different constitutive models to represent the shear band material (where temperature and strain-rate effects are most pronounced) and the surrounding matrix material. Numerical results are presented and compared to experimental data as well as high-resolution conventional FEM results, with the purpose of shedding some light on aspects of shear localization processes which are not yet well-understood, e.g. the importance of softening mechanisms such as dynamic recrystallization, and the dependence of relevant length scales (shear band width) on material and loading parameters.

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Title: Effect of Third Deviatoric Stress Invariant on the Plastic Flow of Al-Alloys

Author(s): Reza Mousavi, Seyedeh Hanie Seyed Joodat, Amir Mohammadipour, *U. Houston* ; Elena Bombasaro, *U. Padova*; Kaspar Willam, *U. Houston*.

A novel asymmetric yield function for metallic materials is proposed depending on the first invariant of the stress tensor and the second and third invariant of stress deviator. This model will be an extension of the three-invariant model for concrete of the senior author when applied to metals and aluminum alloys. The yield function introduces pressure sensitivity and bridges the gap between Tresca and von Mises yield criteria. It is based on experimental observations on aluminum specimens tested under different load scenarios that activate all three tensor invariants. The experimental program includes loading scenarios in which the Lode angle varies from 0 degrees, which corresponds to uniaxial tension and to 30 degrees, and 60 degrees which corresponds to simple shear and uniaxial compression condition. The results can show how the third invariant of stress deviator affects the behavior of the aluminum alloy. Digital Image Correlation (DIC) analysis was used to process full-field measurements of the displacement field and to determine surface strains of the cylindrical aluminum specimen under abovementioned loading scenarios. Using this DIC data, plastic strain measurements were extracted to identify the signature of the three invariants on the plastic flow rule and detect the trace of the first invariant of stress and the second and third invariant of the stress deviator. The results are used to investigate void initiation and growth at the microscopic level of observation. The pressure- sensitivity of the aluminum alloy was further investigated based on the observed failure mode and angle of localization deformations using the DIC images. Analytical and numerical localization analysis are being performed using an associated flow rule in 3D to calculate the orientation of failure surface considering von Mises, Tresca, pressure-sensitive two-invariant formulations and three-invariant formulations. The localization analysis results were compared with the experimental observations and the differences between them are discussed in the presentation.

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Title: On Designing Staggered Coupling Algorithms for Modeling Degradation of Materials

Author(s): Kalyana Nakshatrala, Can Xu, Maruti Kumar Mudunuru, *U. Houston*.

A fundamental study of degradation is crucial to several branches of engineering: aerospace, mechanical, civil, and biomedical. Due to recent advancements in material science, new materials like fiber-reinforced polymers and multi-functional materials that exhibit high ductility have been developed. They have been widely used as infrastructural materials or in medical devices (e.g., stents). Traditional small-strain assumption to model these materials will not be adequate. In this talk, we present a large deformation theory to simulate degradation of materials exposed to inert chemical species. A consistent mathematical model for chemical degradation in hyperelastic solids is presented. The constitutive relations are derived by appealing to the maximization of rate of entropy production. Since the resulting governing equations are coupled non-linear equations, which are not amenable for analytical solutions, we present a robust computational framework to solve the resulting coupled problem based on a staggered coupling approach. The solution procedure consists of solving two sub-problems: deformation of the material and transport of chemical species. The proposed staggered approach is built upon the ideas of Armero and Simo [IJNME, vol. 35, p. 737, 1992]. The predictive capabilities and the robustness of the computational framework will be illustrated using representative numerical examples. At last, we show how degradation affects the dynamic response of hyperelastic solids, and the affect of large strains and large deformations on the transport of the chemical species.

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Title: Embolus Interactions With Blood Flow and Its Role in Stroke

Author(s): Debanjan Mukherjee, Shawn C. Shadden, *UC Berkeley*.

Despite the importance of embolus transport up to the cerebral vasculature in stroke etiology, hemodynamic factors influencing the transport of such particles are not yet well understood. In this work, numerical studies on embolus transport across human carotid bifurcation are performed to i) compare the estimated embolus distribution fractions with and without the incorporation of two-way fluid-particle coupling, and ii) provide deeper insights into hemodynamic factors that play a notable role in embolus transport. We develop a coupled Euler-Lagrange framework for image based CFD to simultaneously compute blood flow velocity and pressure fields, and embolus trajectories. Anatomical model of the bifurcation is constructed from patient Computed Tomography (CT) images. Blood is modeled as an incompressible, Newtonian fluid. Embolic particles are modeled using a modified Maxey-Riley equation, with added contact force function to account for embolus interactions with vessel wall. A simple two-way particle-fluid coupling formulation is employed by augmenting the Navier-Stokes equation with a momentum source due to the particle. Estimates of embolus distribution across the bifurcation are compared between one-way and two-way fluid-particle coupling models. For small to moderate particle sizes relative to vessel diameter, the estimates are found to match reasonably well. The maximum observed differences were found to be higher for idealized bifurcation geometry. Additionally, the distribution reasonably matches the volumetric flow distribution for the idealized case, while a preferential migration of particles to one branch vessel is observed in the anatomical case. Analysis of embolus paths reveal a pronounced swirling flow for emboli traveling across the anatomical bifurcation as compared to the idealized. Local flow helicity is chosen as an appropriate descriptor to elucidate the mechanics of the helical motion. A particle swirl indicator, based on a decomposition of the particle velocity along the centerline tangent and azimuthal directions was used to compare with helicity. Regions of high helicity and high swirl correlate well in general. A lag in the regions of high swirl is observed based on increased particle sizes and momentum response times. Our research indicates that for anatomical geometries, vessel curvature and swirling flow have a dominant effect when compared to the choice of coupling for distribution of small-to-moderate sized emboli. For such cases, one-way coupling is found to be a reasonable approximation. Results indicate that helical flow plays an important role in transporting embolic particles across vasculature segments, which has not been considered in the majority of prior embolic distribution studies.

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Title: Dislocation Dynamics Simulations of Plastic Deformation Near Voids and Precipitates

Author(s): Lynn Munday, Joshua Crone, James Ramsey, Jaroslaw Knap, *Army Rsch. Lab*.

Under hydrostatic loading, dislocations forming prismatic dislocation loops (PDL) produce plastic relaxation through void growth or particle decoherence. In this work, dislocation dynamics simulations are used to characterize two mechanisms for PDL formation. The first mechanism corresponds to a classical model for PDL generation from dislocation nucleation. The second mechanism considers PDL generation from an infinite screw dislocation. The second mechanism corresponds to PDL generation in a lattice containing initial dislocation content. We systematically study the effect of the crystal lattice and defect type on PDL generation for both mechanisms as a function of pressure. The simulations show image stresses produced by the dislocation's interaction with a void will suppress PDL generation. The highest rates of PDL generation are from a dislocation nucleated from a void in a base-centered cubic lattice. The infinite screw dislocations are found to produce a continuous emission of PDLs at pressures as low as 1.0 GPa. Dislocation dynamics simulations are then presented that address the longer term plastic deformation near the defect due to far-field loading conditions. These simulations will include dislocation multiplication of dislocations present in the bulk, a mechanism for dislocation nucleation and the previously discussed mechanisms for PDL generation. These simulations will provide the stress/strain response and the evolving dislocation density. Our simulations use the DD algorithm of van der Geissen and Needleman [1] where the linear elastic fields due to dislocations in an infinite bulk crystal are superimposed onto the linear elastic fields produced by an auxiliary boundary value problem (BVP) whose boundary conditions consist of the corrective image tractions on free surfaces and far-field loads. The BVP also includes corrective body forces due to material inhomogeneities such as precipitates. This simulation protocol is accomplished by coupling the DD simulator ParaDiS [2] to the corrective fields obtained from a BVP solved with a parallel finite element code [3]. This work was supported in part by a grant of high performance computing time from the U.S. Army Research Laboratory DoD Supercomputing Resource Center at Aberdeen Proving Ground, Maryland. [1] E. van der Giessen and A. Needleman, Model. Simul. Mater. Sci. Eng. 3, 689 (1995). [2] A. Arsenlis et al., Model. Simul. Mater. Sci. Eng. 15, 553 (2007). [3] J.C. Crone et al., Model. Simul. Mater. Sci. Eng. 22, 3 (2014).

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Title: New Developments on High-Order Hybridized Discontinuous Galerkin Methods

Author(s): Sriram Murai, Shinhoo Kang, Tan Bui-Thanh, *UT Austin*.

In this talk we will present our new developments on the hybridized discontinuous Galerkin (HDG) methods for partial differential equations: 1) we shall show that HDG methods can be systematically derived using either Godunov method or the Rankine-Hugoniot condition; 2) we present a semi-implicit HDG method for nonlinear equations; 3) we construct an efficient and scalable multi-level HDG solver; 4) we shall present a non-conforming HDG method. Various numerical results will be presented to validate our developments