

Title: A Finite Strain Thermo-Hydro-Mechanical Model for Thermal Softening Geomaterials

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Non-mechanical loadings, such as pore fluid pressure and thermal effects, often influences, the onset and modes of deformation bands. Experimental evidence has established that temperature changes can alter the shape and size of the yield surface, and cause shear band to form in geomaterials that are otherwise stable. Understanding this thermo-hydro-mechanical responses are important for many engineering applications, such as carbon dioxide storage and extraction of hydrocarbon in which hot or cool fluid are often injected into deep porous rock formations. The purpose of this research is to simulate this coupled process using a thermoporoplasticity model with extended hardening rules. A key feature of this model is that evolution of internal variables are governed by both the plastic dissipation and the change of temperature. An adaptively stabilized monolithic finite element model is proposed to simulate the fully coupled thermo-hydro-mechanical behavior of porous media undergoing large deformation. We first formulate a finite-deformation thermo-hydro-mechanics field theory for non-isothermal porous media. The corresponding (monolithic) discrete problem is then derived adopting low-order elements with equal order of interpolation for the three coupled fields. A projection based stabilization procedure is designed to eliminate spurious pore pressure and temperature modes due to the lack of the two-fold inf-sup condition of the equal-order finite elements. To avoid volumetric locking due to the incompressibility of solid skeleton, we introduce a modified assumed deformation gradient in the formulation for non-isothermal porous solids. Finally, numerical examples are given to demonstrate the versatility and efficiency of this model.

Title: Micro-Mechanical Study of High Cycle Fatigue in Polycrystalline Metals Using Energy Method

Author(s): Mehdi Naderi, Mehdi Amiri, Nagaraja Iyyer, *TDA, Inc.*; Nam Phan, *US Naval Air Sys. Comm.*; Peter Kang, *U.S. Naval Air Sys. Comm.*.

An analysis of high cycle fatigue is conducted through the numerical simulation of polycrystalline metals using crystal plasticity finite element method (CPFEM). We presented an approach to estimate the fatigue crack nucleation onset based on crystal plasticity using energy concept. Different representative volume elements containing verities of microstructure morphology and grain sizes are used. Statistically stored dislocation (SSD) and geometrically necessary dislocation (GND) are estimated from crystal plasticity for a double notch specimen. The CPFEM and fatigue damage are implemented in user material subroutine of ABAQUS software and the results are presented for AL 7075-T6. The numerical results of fatigue life are compared with the experimental data available for Al 7075-T6.

Title: Construction of DPG Fortin Operator

Author(s): Sriram Nagaraj, Socratis Petrides, *UT Austin*.

The standard Petrov-Galerkin methodology of solving the variational formulation of second order PDEs often assumes the Babuska inf-sup condition in order to assure the stability of the discrete problem. However, one cannot always guarantee the validity of this assumption. Alternatively, one may choose the test space in an “optimal” fashion in such a way that the discrete formulation for this choice of test space is stable. This point of view can also be interpreted as a mixed formulation as well as a minimum residual formulation. Unfortunately, the “ideal” choice of optimal test functions is computationally intractable, and we replace it with a practical approximation to the ideal test functions. In order to study the effect of using the practical test functions on the stability of the Petrov-Galerkin method, one must construct a continuous map from the infinite dimensional test space to the finite dimensional approximation to the test space. Such a map is called a Fortin operator [1][2]. We highlight the construction of a DPG Fortin operator for H^1 and $H(\text{div})$ spaces, focusing on a uniform triangular 2D mesh. We present sufficient conditions to ensure the uniqueness of the Fortin operator for the H^1 and $H(\text{div})$ cases, using the Helmholtz and acoustic equations respectively as motivation. Further, we develop a numerical procedure to estimate an upper bound on the continuity constant of the Fortin operator in terms of the inf-sup constant γ_h . Our results indicate that the construction of the Fortin operator is feasible, and we estimate the continuity constant of the operator for various choices of the order p and enriched order $p + d_p$ of the trial and test spaces respectively. We see that γ_h decays with increasing p for fixed d_p , and is relatively independent of d_p with fixed $p \geq 3$. References: 1. J. Gopalakrishnan, W. Qiu, “An analysis of the practical DPG method” *Math. Comp.* 83 (2014), 537-552 2. L. Demkowicz, J. Gopalakrishnan “A class of discontinuous PetrovGalerkin methods. Part II: optimal test functions” *Numerical Methods for Partial Differential Equations*, 27 (2010), pp. 70105 3. S. Nagaraj, S. Petrides, L. Demkowicz, “Construction of DPG Fortin Operator”, ICES Report (in preparation)

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Title: Fatigue Crack Propagation Analysis by Three-Dimensional XFEM Considering Penetration Behavior

Author(s): Toshio Nagashima, Kiminori Murai, *Sophia U.*

Fatigue crack propagation analyses for a plate with a semi-elliptical surface crack under repeated tension load are performed by XFEM (the extended finite element method), which can model crack geometry independently of finite elements. Crack front geometry is updated due to stress intensity factors obtained by XFEM analysis and an assumed Paris' law. In this computation, a treatment for a transition from surface crack to penetration crack during crack propagation is considered. Moreover, crack tip elements enriched with only Heaviside function are utilized for XFEM analysis, and the results are compared with conventional XFEM using both Heaviside and asymptotic basis functions.

Title: Computational Statistical Inverse Problems with Sparse or Missing Data

Author(s): Habib Najm, Khachik Sargsyan, Kenny Chowdhary, Mohammad Khalil, *Sandia Nat'l. Lab.*

Statistical inverse problems arise in many important applications, where the estimation of quantities of interest with associated uncertainty estimates is key. In particular, uncertainty quantification in computational models relies on requisite probabilistic characterization of uncertain model inputs, parameters, and operating conditions, which is effectually arrived at by the solution of statistical inverse problems given available data. In this talk, we address specific challenges with the computational solution of statistical inverse problems, related to sparse or missing data. When available data is sparse, some degree of regularization is required to render the inverse problem solvable. Further, and particularly in high-dimensional inverse problems, it is important to discover and make use of sparsity in the fitted-model, employing regularization with l_1 constraints. We outline our recent work in this context, focusing on Bayesian compressive sensing, where we use Laplace priors for regularization. We illustrate application of this technique in the context of land components of climate models. Alternatively, in many practical situations, actual data is simply not available, and one is limited to available data summaries, in the form of statistics, such as nominal values and conditional/marginal bounds, on the quantities of interest or functions thereof. Maximum entropy (MaxEnt) methods are useful for inference employing constraints, rather than data. I will describe our computational implementation of the MaxEnt principle employing approximate Bayesian computation methods, to enable inference of uncertain parameters given summary statistics. I will present illustrations of the performance of this construction in model problems.

Title: Optimization of Communications for Scalable Algorithms on Supercomputers in Next Generation

Author(s): Kengo Nakajima, *U. Tokyo.*

Parallel multigrid method is expected to be a powerful tool for large-scale computations, but includes both of serial and parallel communication processes which are generally expensive. The serial communication is the data transfers through memory hierarchies of each processor, while the parallel one is by message passing between computing nodes using MPI. This presentation summarizes recent efforts of optimization of serial and parallel communications in parallel MGCG (conjugate gradient with multigrid preconditioning) solvers with geometric multigrid procedures using up to 4,096 nodes (65,536 cores) of Fujitsu PRIMEHPC FX10 [1]. Performance of both of flat MPI and HB MxN (M: number of threads on each MPI process, N: number of MPI processes on each node) has been evaluated. In the present work, new format for sparse matrix storage based on sliced ELL, which has been well-utilized for optimization of SpMV, is proposed for optimization of serial communication on memories, and hierarchical coarse grid aggregation (hCGA) is introduced for optimization of parallel communication by message passing. The parallel MGCG solver using the sliced ELL format provided performance improvement in both weak scaling (25%–31%) and strong scaling (9%–22%) compared to the code using the original ELL format. Moreover, hCGA provided excellent performance improvement in both weak scaling (1.61 times) and strong scaling (6.27 times) for flat MPI parallel programming model. hCGA was also effective for improvement of parallel communications. Computational amount of coarse grid solver for each core of flat MPI is 256 (=16x16) times as large as that of HB 16x1. Therefore, hCGA is expected to be really effective for HB 16x1 with more than 2.50×10^5 nodes of Fujitsu FX10, where the peak performance is more than 60 PFLOPS. CGA and hCGA include a various types of parameters, and the optimum values of those were derived through empirical studies in the present work. Development of methods for automatic selection of these parameters is also an interesting technical issue for future work. Optimum parameters can be estimated based on calculation of computational amounts, performance models, parameters of hardware, and some measured performance of the system. But it is not so straightforward. Because some of these parameters also make effects on convergence, construction of such methods for automatic selection is really challenging. [1] Nakajima, K., Optimization of Serial and Parallel Communications for Parallel Geometric Multigrid Method, Proceedings of the 20th IEEE International Conference for Parallel and Distributed Systems (ICPADS 2014) (2014) 25-32

Title: A Christoffel Function Weighting Algorithm for Least-Squares Collocation Approximation

Author(s): Akil Narayan, *U. MA Dartmouth*; John Jakeman, *Sandia Nat'l. Labs.*; Tao Zhou, *Chinese Acad. Sci.*.

Monte Carlo methods for the construction of least-squares polynomial approximations are effective tools for computing a parameterized model surrogate. We propose and investigate an algorithm for a particular kind of weighted Monte Carlo approximation method that we call Christoffel Least Squares (CLS). With an expansion in an orthogonal polynomial basis, a standard Monte Carlo approach would draw samples according to the density of orthogonality. Our proposed CLS method samples with respect to the (weighted) equilibrium measure of the parametric domain, and subsequently solves a weighted least-squares problem, with weights given by evaluations of the Christoffel function. We present theoretical analysis to motivate the algorithm, and numerical results that show our method is superior to standard Monte Carlo methods in many situations of interest.

Title: Investigation of Flow Corrective Devices for the Heat Recovery Steam Generation Inlet Duct

Author(s): Farooq Nasser Al-Jwesm, *Saudi Aramco*.

In this study, the flow corrective devices for the heat recovery steam generation inlet duct were investigated. The flue gas in inlet duct goes through a sudden expansion at a rate of 475 kg/s prior impinging on the super heater tubes bank for the heat recovery steam generator. Computational Fluid Dynamics techniques were used to simulate the flow behaviour in the inlet duct. The simulation revealed that installation of flow corrective devices is essential to produce a uniform flow pattern at the duct exit. The purpose of this study is to produce homogenised flow at the outlet of the inlet duct to avoid possible hot spots on the tubes bank and back pressure on the gas turbine. The effect of perforated plate, flow diverter and baffles on homogenising the flow was studied. Also, this study proposed a new flow corrective device that will have minimum pressure drop with little modification on the inlet duct for heat recovery steam generator. The results of this study have shown that using flow corrective devices will significantly enhance the flow upstream of the super heater tubes bank. However, each device is associated with different pressure drop and velocity RMS at the outlet of the inlet duct. Hence, optimum selection for flow corrective devices depends on the heat recovery steam generator allowable pressure drop and RMS value. The simulation results were compared and validated with the previous results available in the literature.

Title: Study of the Biomechanical Behavior of the Female Bladder Neck

Author(s): Renato Natal Jorge, Marco Parente, Dulce Oliveira, Elisabete Silva, *U. Porto*; Sofia Brandão, Teresa Mascarenhas, *Centro Hospitalar de Sao Joao-EPE*.

The female pelvic floor is an understudied region of the body from the biomechanical perspective. MRI has been used in the diagnostic evaluation of the pelvic floor dysfunctions. Static images show their morphology while dynamic images show the functional changes that occur on straining and contraction of the pelvic floor. In the present work, MR images contribute to generate 3D solids of pelvic floor muscles through manual segmentation. To study the biomechanical behavior of pelvic floor muscles the Finite Element Method (FEM) would be applied to these 3D solids, contributing to analyze this complex musculature structure [1]. The purpose of this work was to model the bladder neck mobility for valsalva maneuver, taking into account progressive impairment of the pelvic ligaments. This was performed taking into account live subject data and a computational model based on the Finite Element Method. Multiplanar pelvic high-resolution T2w Magnetic Resonance images were acquired in the supine position at rest using a 3T scanner. Additional dynamic images during valsalva maneuver were obtained in the sagittal plane. The high-resolution T2w images were used to identify and segment several anatomical structures (the pelvic bones, organs and several soft tissue support structures were included). The organs were described as having hyperelastic mechanical behaviour while the bones were fixed and considered as rigid. All the structures were exported in step format to the FE analyses software ABAQUS. The present study showed the predicted motion of the urethra and bladder neck during valsalva maneuver, for both healthy and impaired ligaments. Acknowledgments The authors acknowledges the founding of the project "LAETA - UID/EMS/50022/2013" from Ministério da Educação e Ciência, FCT, Portugal. References [1] S Brandão, MPL Parente, T Mascarenhas, ARG Silva, I Ramos, RM Natal Jorge, "Biomechanical study on the bladder neck and urethral position: simulation of impairment of the pelvic ligaments", *Journal of Biomechanics*, 48:217-223, 2015.

Title: Numerical Studies on the Role of Stress-Diffusion Interactions on the Fracture and Crack Growth in Lithium Ion Battery Electrode Particles Using the Extended Finite Element Method

Author(s): Kate Aifantis, *U. Arizona*; Sundararajan Natarajan, *Indian Inst. Tech.-Madras*; Narasimhan Swaminathan, Ratnakumar Annabatula, *Indian Inst. Tech-Madras*.

In this paper, we study the effects of stress-diffusion interactions on the fracture behavior and the crack growth in Lithium ion battery electrode particles. A coupled mechanical equilibrium and Lithium diffusion which accounts for the effect of stresses on diffusion and the effect of advancement of the front to the crack growth is considered. The discontinuous fields are represented independent of the mesh within the framework of the XFEM and linear elastic fracture mechanics is used to analyze the crack growth behavior. The advancing front is represented by the level sets and the stress distribution and the fracture parameters are estimated to understand the effect of coupling during lithiation. The fracturing is simulated based on the maximum principal stress criterion. The numerical results are compared with available experimental results. The proposed framework will provide insights into understanding the failure and degradation of the electrodes under potentiostatic and galvanostatic conditions. The influence of the particle size and shape on the fracture parameters and the stress distribution is also investigated.

Title: DG-FTLE: Lagrangian Coherent Structures with High-Order Discontinuous-Galerkin Methods

Author(s): Daniel Nelson, Gustaaf Jacobs, *San Diego State U..*

We present an algorithm for the computation of finite-time Lyapunov exponent (FTLE) fields using discontinuous-Galerkin (DG) methods in two dimensions. The algorithm is designed to compute FTLE fields simultaneously with the time integration of DG-based flow solvers of conservation laws. Fluid tracers are initialized at Gauss-Lobatto quadrature nodes within an element. The deformation gradient tensor, defined by the deformation of the Lagrangian flow map in finite time, is determined per element with high-order DG operators. Multiple flow maps are constructed from a particle trace that is released at a single initial time by mapping and interpolating the flow map formed by the locations of the fluid tracers after finite time integration to a unit square master element and to the quadrature nodes within the element, respectively. The interpolated flow maps are used to compute forward-time and backward-time FTLE fields at several times using DG operators. For a large finite integration time, the interpolation is increasingly poorly conditioned because of the excessive subdomain deformation. The conditioning can be used in addition to the FTLE to quantify the deformation of the flow field and identify subdomains with material lines that define Lagrangian Coherent Structures. The algorithm is tested on three benchmarks: an analytical spatially periodic gyre flow, a vortex advected by a uniform inviscid flow, and the viscous flow around a square cylinder. In these cases, the algorithm is shown to have spectral convergence.

Title: MaMiCo: Software Design for Coupled Massively Parallel Molecular-Continuum Flow Simulations

Author(s): Philipp Neumann, Nikola Tchipev, Hans-Joachim Bungartz, *Tech. U. München.*

The behavior of fluids significantly deviates from continuum law descriptions when the characteristic length of the considered scenario approaches the molecular scale. This particularly holds for fluid motion close to surfaces, in nanosized devices such as nanofilters, or in nano-channels. A numerical method capable of simulating any of these cases needs to account for the interaction of fluid molecules with the walls/geometry. Pure molecular dynamics (MD) simulation methods may become very expensive in complex flow simulations at the nanoscale. Hybrid molecular-continuum methods have become a popular means for the investigation of nanofluidics, yielding accurate results at acceptable computational cost. Over the last years, we have developed the macro-micro-coupling tool MaMiCo to provide a flexible, modular and parallel piece of software to couple mesh-based flow solvers and molecular dynamics simulations for fluid dynamics applications [1]. We demonstrate functionality and performance of the tool by coupling four molecular dynamics codes to the spatially adaptive Lattice Boltzmann (LB) solver waLBerla (URL walberla.net): SimpleMD, ls1 mardyn (URL ls1-mardyn.de), ESPResSo (URL espressomd.org) and LAMMPS (URL lammps.sandia.gov). SimpleMD represents a simple test environment for single-centered Lennard-Jones simulations. ls1 mardyn is a molecular dynamics simulation software, developed as part of a collaboration between process engineers and computer scientists. It targets large (massively parallel) systems arising in chemical engineering and broke the record for the largest MD simulation in 2013 by simulating more than four trillion molecules [2]. ESPResSo and LAMMPS represent powerful open-source frameworks for the parallel simulation of many-particle systems such as atomistic, coarse-grained or colloidal systems. We discuss the MaMiCo interface implementations and validate them by considering a state-based molecular-continuum simulation of channel flow. We further provide strong scaling results for different simulation scenarios and show preliminary studies of more complex nanoflow scenarios. [1] Neumann, P., Tchipev, N., A Coupling Tool for Parallel Molecular Dynamics-Continuum Simulations, Proceedings of the International Symposium on Parallel and Distributed Computing, 2012. [2] Eckhardt, W., Heinecke, A., Bader, R., Brehm, M., Hammer, N., Huber, H., Kleinhenz, H.-G., Vrabec, J., Hasse, H., Horsch, M., Bernreuther, M., Glass, C., Niethammer, C., Bode, A., Bungartz, H.-J., 591 TFLOPS Multi-Trillion Particles Simulation on SuperMUC, International Supercomputing Conference Proceedings 2013, Springer, 2013.

Title: Computational Geomechanics of CO₂ Geological Storage Systems

Author(s): Pania Newell, Mario J. Martinez, *Sandia Nat'l. Lab.*

Geological sequestration of CO₂ refers to the process of injecting carbon dioxide (CO₂) into deep subsurface saline aquifers for long-term storage. The injected buoyant CO₂ is trapped beneath a low-permeability caprock formation. Maintaining caprock integrity during the injection process is the most important factor for a successful injection. However, there are pre-existing fractures within most caprock formations. In this work, we evaluate the integrity of the jointed/fractured caprock during injection scenarios using coupled three-dimensional multiphase flow and geomechanics modeling. Evaluation of jointed/fractured caprock systems is of particular concern to CO₂ sequestration because creation or reactivation of joints can lead to enhanced pathways for leakage. In this work, we adopt an equivalent continuum approach to account for the joints within the caprock. Based on the effective normal stress, the joint aperture and non-linear stiffness of the caprock will be updated dynamically. The effective permeability field will also be updated based on the local joint aperture, leading to an anisotropic permeability field within the caprock. This feature adds another coupling mechanism between the solid and fluid in addition to basic Terzaghi effective stress concept. In this study, we evaluate the impact of the geometry of caprock and reservoir layers on geomechanical response of the geological system during CO₂ sequestration operations. 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.

Title: A Fully-Implicit Approach to Phase-Field Modeling of Dendritic Solidification

Author(s): Chris Newman, Marianne Francois, *Los Alamos Nat'l. Lab.*

We examine a fully-coupled, fully-implicit approach to phase field modeling of dendritic solidification. Modeling of dendrite growth in pure metals and alloys remains a significant challenge in the field of materials science, as micro-structure formation during the solidification of a material plays an important role in the properties of the solid material. The distinguishing characteristic of the phase field approach is that the interface between phases is diffuse. In contrast to methods which assume a sharp interface between phases, the phase field approach avoids explicit tracking of this interface. Explicit time discretizations can be impractical due to short timesteps restricted by CFL conditions. One of the direct advantages of implicit methods is that large, second order timesteps can be taken. A disadvantage however, is that fully implicit methods require a nonlinear solution be attained for each timestep. Our approach consists of a finite element spatial discretization of the fully-coupled nonlinear system, which is treated implicitly with a preconditioned Jacobian-free Newton-Krylov (JFNK) method. The key to efficient implementation of JFNK is effective preconditioning. As the dominant cost of JFNK is the linear solver, effective preconditioning reduces the number of linear solver iterations per Newton iteration. We discuss a preconditioning strategy based on algebraic multigrid and block factorizations that allows an efficient, implicit time integration. We provide numerical examples and compare our method to explicit methods to evaluate efficiency, accuracy and algorithmic scalability.

Title: Phase Field Modelling of Complex Microcracking in Voxel-Based Models of Cementitious Materials

Author(s): Thanh Tung Nguyen, Julien Yvonnet, Qi Zhi Zhu, Michel Bornert, Camille Chateau, *U. Paris-Est.*

PHASE FIELD MODELLING OF COMPLEX MICROCRACKING IN VOXEL-BASED MODELS OF CEMENTITIOUS MATERIALS
Key Words: Cracks, Phase field, Voxel-based models, Microcracking, Heterogeneous materials.
Abstract: In this work, a numerical technique based on the phase field method is proposed to model complex microcracking in voxel-based models of cementitious materials obtained from micro-tomography images. The Phase field method [1], based on a variational formulation of brittle fracture with regularized approximation of discontinuities [2,3], does not require an explicit tracking of the cracks, avoids the classical mesh sensitivity issues related to smeared cracks models. The method employs a diffuse approximation for both interfaces and cracks, and is thus well adapted to voxel-based models of microstructures obtained from X-ray CT images. To describe interfaces, a new method is introduced to construct level-set functions for arbitrary geometries of inclusions in voxel models. The technique allows nucleation of multiple cracks and the modeling of their interactions in complex heterogeneous materials. Several benchmarks are presented to validate the model and the technique is illustrated through numerical examples involving complex microcracking in X-ray CT image-based models of microstructures in cementitious materials. REFERENCES [1] C. Miehe, M. Hofacker and F. Welschinger. A Phase Field model for rate-independent crack propagation. *Computer Methods in Applied Mechanics*, 199:2765-2778 (2010) [2] A.A. Griffith, The phenomena of rupture and flow in solids, *Philosophical Transactions of the Royal Society London A*, 221:163-198 (1921) [3] B. Bourdin, G.A. Francfort, J.J. Marigo, *The Variational Approach to Fracture*, Springer Verlag, Berlin, (2008)

Title: Gaussian Functional Regression for Output Prediction with Mathematical Models and Physical Observations

Author(s): Cuong Nguyen, Jaime Peraire, *MIT*.

We introduce a new statistical regression method to predict an output of interest of a parametric physical system as a function of input parameters. The input-output relationship is mathematically characterized by a linear functional of the solution of a parametrized linear partial differential equation (PDE). In most practical applications, however, the parametrized linear PDE is only an approximate mathematical model due to both the deliberate mathematical simplification of the model to make it tractable, and the inherent uncertainty of model parameters. As a result, the output of the parametrized linear PDE model may be drastically different from the true output of the underlying physical system. To remedy this problem, we propose a Gaussian functional regression method that combines the parametrized linear PDE model with available observations to improve the prediction of the true output. Our method is devised as follows. First, we augment the PDE model with a random functional to represent various sources of uncertainty in the model. This functional is characterized as a Gaussian functional with a mean functional and a covariance operator. We next develop a functional regression procedure to determine the posterior distribution of the Gaussian functional by utilizing observations and adjoint states. It allows us to compute the posterior distribution of the output estimate. Furthermore, we propose new families of covariance operators and develop an algorithm for choosing an appropriate covariance operator based on the observations. We demonstrate the proposed methodology with several numerical examples.

Title: Node-Based Mesh Generation and Adaptive Finite Element Methods

Author(s): Yufeng Nie, *Northwestern Polytech'l. U.*

In accordance with the desired nodal density and the Second Newton's Law of dynamics, automatic generation of nodes set by bubble simulation has been demonstrated. Since the interaction force between nodes is short-range force, for two distant nodes, their positions and velocities can be updated simultaneously and independently during dynamic simulation, which indicates the inherent property of parallelism, it is quite suitable for parallel computing. The results of numerical examples show that quasi liner speedup in the number of processors and high efficiency are achieved. Then a new mesh adaptive algorithm that combines a posteriori error estimation with bubble-type local mesh generation (BLMG) strategy for elliptic differential equations is proposed. The size function used in the BLMG is defined on each vertex during the adaptive process based on the obtained error estimator. In order to avoid the excessive coarsening and refining in each iterative step, two factor thresholds are introduced in the size function. The advantages of the BLMG-based adaptive finite element method, compared with other known methods, are given as follows: the refining and coarsening are obtained fluently in the same framework; the local a posteriori error estimation is easy to implement through the adjacency list of the BLMG method; at all levels of refinement, the updated triangles remain very well shaped, even if the mesh size at any particular refinement level varies by several orders of magnitude. Several numerical examples with singularities for the elliptic problems, where the explicit error estimators are used, verify the efficiency of the algorithm. The analysis for the parameters introduced in the size function shows that the algorithm has good flexibility. Keywords: node placement; molecular dynamics simulation; error estimate; size function;adaptive

Title: Aerodynamic Design for Unsteady Flows Using An Adjoint Approach

Author(s): Eric Nielsen, *NASA* ; Boris Diskin, *Nat'l. Inst. Aerospace*.

A discrete adjoint-based design methodology for unsteady turbulent flows on three-dimensional dynamic overset unstructured grids is described. The methodology supports both compressible and incompressible flows and is amenable to massively parallel computing environments. The approach provides a general framework for performing highly efficient and discretely consistent sensitivity analysis. Meshes consisting of mixed-element topologies and overset component grids are supported, where grids may be static, dynamic, or deforming, including any combination thereof. An overview of a broad range of aerospace applications for which the implementation has been demonstrated will be shown.

Title: Benchmark Computations with High-Order, Shell-Finite Elements

Author(s): Antti H. Niemi, *Aalto U.*

In the finite element modelling of shell structures parametric error growth, or locking, is detected for various shell deformation types. This numerical phenomenon is especially harmful for the standard lowest-order ($p=1$) finite element approximation and significant mesh over-refinement is sometimes needed to compensate for the effect. However, the level of error amplification does not depend on the degree of the approximating polynomials used in the FE approximation and considerably milder mesh over-refinement is needed at higher values of p . Another long-standing approach to modelling of thin structures is the derivation of special low-order formulations that avoid the parametric error growth. For shells, the ultimate dream element is yet to be found but there exist reduced strain formulations that work quite well on restricted class of meshes, at least. In this work, we compare the relative accuracy and efficiency of high order shell formulations and state of the art reduced strain elements in challenging benchmark tests featuring different shell deformation types.

Title: Fully Coupled Phase-Field and Elasto-Viscoplastic Fast Fourier Transform Models for Advanced Mesoscale Thermal-Mechanical Processing Simulation

Author(s): Pengyang Zhao, Yunzhi Wang, Thaddeus Low, Stephen Niezgoda, *Ohio State U.*

Many time-dependent deformation processes at elevated temperatures produce significant concurrent microstructural changes that could alter mechanical properties in a profound manner. Such microstructure changes are usually missing in crystal plasticity or other purely mechanical modeling. Although efforts have been made on developing microstructure-aware crystal plasticity models, the microstructure evolution is essentially still an auxiliary local constitutive law. Here we present an integrated full-field modeling scheme that couples the mechanical response with the underlying microstructure evolution. Based on the seminal work of Moulinec and Suquet and recent extension by Lebensohn and colleagues, fast Fourier transform based methods have become a popular approach for the computation of the complete micromechanical fields in heterogeneous materials. On the other hand, the phase-field method is a well-known methodology for the simulation of the evolution of microstructural fields under a thermodynamic driving force. Here we present a fully coupled simulation framework for thermal-mechanical processing which simultaneously updates the local mechanical (stress/strain rate) fields and evolves the local microstructure (grain growth, phase separation etc). The algorithm is formulated in such a way that the Green's function integrals can be cast as convolution with kernel operators that can be efficiently solved by spectral approaches. Since both methods are image-based and built on Green's function solutions for stress equilibrium and strain compatibility using an identical spectral formulation, datasets generated by one method can be used directly by the other as simulation RVEs, eliminating the difficult and time consuming meshing step that would be required for coupling via finite element. As a first demonstration, we integrate a FFT based elasto-viscoplasticity (FFT-EVP) model with a phase-field (PF) recrystallization model, and apply to 3D simulation of dynamic recrystallization (DRX) in polycrystalline copper. A physics-based methodology interface between FFT-EVP and PF is achieved by (1) adopting a dislocation-based constitutive model in FFT-EVP, which allows the predicted dislocation density distribution to be converted to a stored energy distribution and passed to PF, and (2) implementing a stochastic nucleation model based on local dislocation density for DRX. We demonstrate that this integrated model can faithfully reproduce the experimental stress-strain curves and allow us to study DRX with full-field information.

Title: A Finite-Element Formulation for Curved Thin-Walled Beams

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

Curved beams are widely used in engineering structures such as railway bridges and highway interchanges. When a vertical out of plane loading is applied to a horizontally-curved beam, it undergoes torsion, compression and biaxial moments as primary actions and second order bending moments and torsional moments which occur as a result of coupling between different modes of deformations. In this study, a finite element formulation is developed for thin-walled curved beams made of isotropic material. The beam is assumed to be initially curved in a single plane, and the cross-section is assumed to remain rigid. The formulation is made applicable for beams undergoing large deformations. Firstly, by using Frenet-Serret formulae, the twist and the beam curvatures in x and y directions for the deformed configuration are obtained in terms of the displacement components and the initial curvature. Then, the finite strain values are calculated using right extensional strain definition. At this stage, the stresses are obtained from the strain components by assuming linear elastic material response. Using the principle of virtual work, the nonlinear equilibrium equations are obtained and then linearized to develop the finite element formulation. Due To due aforementioned couplings that exist between the displacement fields, the conventional interpolation functions are replaced by the direct results from the solution of the set of governing differential equations. Numerical examples are performed, and the results are compared with the results in the literature and those of shell finite element modelling in order to validate the accuracy of the proposed model. It can be observed that the current model is accurate for comparatively large included angle per element. References Erkmen, R.E. & Bradford, M.A. 2009, 'Nonlinear elasto-dynamic analysis of I-beams curved in-plan', International Journal of Structural Stability and Dynamics, vol. 9, no. 2, pp. 213-41. Pi, Y.L. & Trahair, N.S. 1997, 'Nonlinear elastic behavior of I-beams curved in plan', Journal of Structural Engineering, vol. 123, no. 9, pp. 1201-9.

Title: Mechanics of Weakly-Bonded Incommensurate Atomic Bilayers

Author(s): Ilia Nikiforov, Ellad Tadmor, *U. Minnesota.*

Using theoretical analysis and computations, we consider the mechanics of weakly-bonded incommensurate bilayers (WIBs). If a WIB is assumed to remain flat and deform affinely, its interlayer binding energy and elastic modulus are identical to a continuum bilayer with appropriate particle densities. If, on the other hand, the atoms are allowed move freely, a free-standing WIB adopts a statically rippled configuration. This out-of-plane rippling is directly caused by the interlayer interactions between incommensurate atoms and is distinct from the rippling observed in free-standing monolayers. The rippling can be treated analogously to the continuum treatment of the Frenkel-Kontorova (F-K) model and shows excellent agreement between the analytical continuum prediction and atomistic simulation.

Title: Enhanced Non-Linear, Finite-Volume Scheme for Multi-Phase Flows

Author(s): Kirill Nikitin, Yuri Vassilevski, *INM RAS*; Vasiliy Kramarenko, *MIPT*; Kirill Terekhov, *Stanford U.*

We present an application of the nonlinear monotone finite volume method to multiphase flow models [1] and the latest enhancement of the method for near-well regions. We consider full anisotropic discontinuous permeability tensors on conformal polyhedral meshes. The approximation of the Darcy flux uses the nonlinear two-point stencil which reduces to the conventional two-point flux approximation (TPFA) on cubic meshes. We show that the quality of the discrete flux in a reservoir simulator has great effect on the front behavior and the water breakthrough time. We compare conventional linear and new nonlinear two-point flux approximations, and linear multi-point flux approximation (MPFA). The nonlinear monotone scheme has a number of important advantages over the traditional linear discretizations. Compared to the linear TPFA, the nonlinear scheme demonstrates low sensitivity to grid distortions and provides appropriate approximation in case of full anisotropic permeability tensor. For non-orthogonal grids or full anisotropic permeability tensors the conventional linear TPFA provides no approximation, while the nonlinear flux is still first-order accurate. The computational work for the new method is higher than the one for the conventional TPFA, yet it is rather competitive. Compared to MPFA, the nonlinear scheme provides sparser algebraic systems and thus is less computationally expensive. Moreover, it is monotone which means that the discrete solution preserves the non-negativity of the differential solution. The latest enhancement of the nonlinear method takes into account the logarithmic behavior of the pressure in the near-well region and introduces logarithmic correction to improve accuracy of the pressure and the flux calculation. [1] K.D.Nikitin, K.M.Terekhov, Y.V.Vassilevski, "A monotone nonlinear finite volume method for diffusion equations and multiphase flows" // Computational Geosciences: Vol. 18, No. 3, (2014), pp 311-324, DOI: 10.1007/s10596-013-9387-6.

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Title: Development, Validation and Application of Simulation Capabilities for Hydraulic-Driven Fracture Propagating in Porous Medium

Author(s): Jing Ning, Matias Zielonka, Gilbert Kao, Garzon Jorge, Nikolay Kostov, Kevin Searles, Scott Buechler, Pablo Sanz Rehermann, *ExxonMobil*.

The problem of a hydraulically driven fracture propagating in a porous medium is studied from different aspects of development, numerical and experimental validation, and business applications for a diverse set of oil & gas problems. Numerical models utilize coupled pressure/deformation cohesive zone elements and extended finite elements to simulate the fracture propagation and fracturing fluid flow which are recently developed modeling capabilities in Abaqus SIMULIA®. The formulations of the two different approaches are discussed and validated against well-known analytical solutions in dimensionless space where extreme values of rock and fluid properties and leak-off conditions are considered. Additionally, experimental validation is carried out by comparing the predicted injection pressure and final fracture and leak-off geometry from numerical models with lab measurements. The well-matched results provide confidence in the numerical ability to accurately model field-scale fluid driven fracturing applications including drilling wellbore integrity lost returns, drill cuttings disposal, long-term water injection, and hydraulic fracture stimulation. Successful modeling of these business applications with large length scales and long time-scales using extensive 3D models and high-performance parallel computing systems demonstrate a new approach for solving complex hydraulic fracturing problems.

Title: Simulation of Elastic Wave Propagation Using Cellular Automata and Peridynamics

Author(s): Vinesh Nishawala, Martin Ostoj-Starzewski, *U. Illinois, Urbana-Champaign*; Michael Leamy, *Georgia Inst. Tech.*; Paul Demmie, *Sandia Nat'l. Lab.*

Peridynamics is a non-local continuum mechanics formulation that can handle spatial discontinuities as the governing equations are integro-differential equations which do not involve spatial gradients. Cellular automata is a local computational method which is mathematically equivalent to the central difference finite difference method of classical elasticity, but does not require the derivation of the governing partial differential equations. Bond-based peridynamics and cellular automata are used to solve a homogeneous half-space subjected to a normal line load, known as Lamb's problem. Lamb's problem can be used to model the survivability of surface and underground structures. A surface correction methodology to the peridynamics formulation is applied and mesh convergence data are provided. Location and magnitude of the pressure, shear and Rayleigh waves for each method are evaluated. The surface response of each method is compared to the theoretical solution from classical elasticity and existing experimental, photoelastic results. We find that cellular automata, peridynamics, and theoretical results follow closely. Additionally, spatial randomness is introduced in the mass distribution of the system and a quantitative parameter sensitivity study using Lamb's problem is conducted. References [1] Silling, S.A., 2000. "Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces". *J. Of the Mech. and Phys. of Solids*. 48, 175-209. [2] Leamy, M.J., 2008. "Application of Cellular Automata Modeling to Seismic Elastodynamics". *Int. J. of Solids*. 45, 4835-4849. [3] Dally, J.W., 1967. "Observations of Stress Wave Propagation in a Half-plane with Boundary Loading". *Int. J. Solids Structures*. 3, 293-308.

Title: Optimal Design of In-Plane Unit in Composite Plates

Author(s): Shin-nosuke Nishi, Shinsuke Takase, Junji Kato, Kenjiro Terada, *Tohoku U.*

The present study proposes topology optimization method of in-plane unit cells that maximizes the overall mechanical performance of composite plates. Here, an in-plane unit cell is defined as a structural unit of periodic microstructures arranged to form a composite plate, and determines not only the in-plane stiffness but also the out-of-plane bending, torsion and shear stiffnesses. The proposed optimization method is based on the two-scale composite plate model, which has recently formulated to characterize the macroscopic plate stiffness within the framework of mathematical homogenization theory. In this two-scale model, a thick plate theory is employed at macro-scale, while three-dimensional solids are assumed at micro-scale. The macroscopic plate stiffnesses are obtained via the numerical plate testing (NPT), for which we solve the microscopic boundary value problem (BVP) that is consistent with the macroscopic BVP for a homogenized thick plate. To determine the optimal material layout in an in-plane unit cell, the design variable for the optimization method is assumed to be the volume fraction of constituent material in each finite element of the corresponding finite element model. The relevant sensitivity analysis is performed to update all the design variables in the unit cell model. In this particular study, the optimality criteria method (OC) or the method of moving asymptotes (MMA) is employed as an optimizer with the evaluated sensitivities. Two optimization problems are set up in this study. The first one is the so-called inverse homogenization, in which we obtain the topologies of unit cells that provides pre-defined values of the plate stiffness. That is, we perform NPTs for a unit cell with simple material layout to calculate the corresponding plate stiffness, and then try to obtain the pre-defined unit cell with an appropriate objective function. Several numerical examples are presented to verify the capability of the proposed method with the employed two-scale model. The other one is topology optimization for a unit cell that maximizes some components of the macroscopic plate stiffness subjected to some patterns of macroscopic deformations in NPTs. For instance, the optimal cross-section structure of a sandwich panel can be designed so as to maximize the out-of-plane-shear stiffness with some constraints for large bending rigidity. Several optimized structures with their homogenized plate stiffness matrices are presented to demonstrate the capability of the proposed topology optimization method.

Title: Stability, Buckling and Postbuckling Analysis of Curved Panels

Author(s): Mihaela Nistor, Yang Zhou, Ilinca Stanciulescu, *Rice U.*

Aerospace, mechanical and civil engineering systems widely make use of curved panels as structural components. The curved panels exhibit high risk of loss of stability especially with the requirements for increasingly lighter designs. Correct identification of the load-carrying capabilities and thorough understanding of the full equilibrium manifold provide necessary information to safely design such structural components. Buckling and postbuckling analysis of curved panels has been the focus of many researchers. A variety of numerical approaches are available in the literature for such analysis. In this work the numerical procedure chosen uses the arclength and branch-switching methods. Previous studies have either overestimated the buckling load and identified a false buckling mode, or failed to identify all secondary solution branches. Compared to other methods available the chosen method does not require prior knowledge of the bifurcation modes and uses the same mesh for tracing all secondary paths of the structure. Also, the method has identified secondary branches that other procedures failed to retrieve. In the adopted procedure the primary equilibrium path is traced by the arc-length method while monitoring the lowest eigenvalues of the tangent stiffness matrix. All critical points (limit and bifurcation points) on the primary path are found by identifying all zero eigenvalues. The multiplicity of zero eigenvalues differentiates the bifurcation points into simple or multiple. The switch from the primary path to a secondary path at a bifurcation point is achieved through a branch-switching method while the remaining solutions on the secondary path are traced using the arclength method. If another secondary path is present, a restart option is used to go directly to the bifurcation point where branch-switching method is performed again followed by arclength method. Orthogrid panels are known to have superior strength and stiffness-to-weight ratios. These properties make them attractive for use as structural components. However, their stability is far from being well-understood. In this talk, the influence of various geometrical parameters of the curved orthogrid panels on the full equilibrium manifold is discussed. Also, a comparison highlighting the differences between responses of curved panels and orthogrid curved panels is presented.

Title: An Enriched Conformal Decomposition Finite Element Method with Guaranteed Quality

Author(s): David Noble, Richard Kramer, *Sandia Nat'l. Lab.*

Enriched finite element methods such as the Conformal Decomposition Finite Element Method (CDFEM) are powerful tools for multiphase and multimaterial problems. To accurately capture interfacial physics and discontinuities, these methods provide discretizations that dynamically adapt to moving material and phase boundaries by introducing enrichment in elements crossed by the interfaces. Additional unknowns are assigned to one or more of the mesh entities (elements, nodes, edges, or faces) that are associated with these interfacial elements, and additional equations are formulated for these unknowns. Care must be taken in all enriched finite element methods to ensure that the resulting system of equations is well conditioned. As an interface can come arbitrarily close to background mesh nodes, the equations for the added degrees of freedom may become linearly dependent on the equations for the existing degrees of freedom. To handle this issue, practitioners have omitted the enrichment in elements that intersect only a small fraction of the additional material [1]. Poor conditioning can thereby be limited by snapping the interface to the nearest background mesh node when a minimum separation is reached. However, this snapping introduces an error in the location of the interface. An alternate approach is presented that removes the poor conditioning without introducing an error in the interface location. When an edge is crossed by the interface near one of its ends, the nearest node of the edge is moved to the crossing instead of moving the crossing to the node. This method is similar to that used in Isosurface Stuffing [2], which produces meshes that conform to an isosurface with guaranteed quality. Because this process does not introduce any error in the interface location, larger snapping tolerances can be used to produce high accuracy and robustness. The method is shown to improve the quality of the decomposed meshes and dramatically improve the conditioning of the resulting system of equations. *Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000. REFERENCES [1] Moës N, Gravouil A, Belytschko T. Non-planar 3D crack growth by the extended finite element and level sets—part I: Mechanical model. *International Journal for Numerical Methods in Engineering* 2002; 53:2549–2568. [2] Labelle F and Shewchuk JR, Isosurface Stuffing: Fast Tetrahedral Meshes with Good Dihedral Angles, *ACM Transactions on Graphics* 26(3):57.1-57.10, 2007

Title: Stability Analysis of Arches on an Elastic Foundation

Author(s): Christianne Nogueira, *Federal U. Ouro Preto*; Ricardo Silveira, *Federal U. Ouro Preto* ; Paulo Gonçalves, *Pontifical Catholic U. Rio de Janeiro* .

Structural elements such as arches, beams and plates are used in order to transferring load from super-structure to the geological medium. Initially resting on the geological medium, those elements can loose the contact during the deformation process due to its incapability of reacting under tension, leading to important difference in the foundation's reaction and internal stresses in the structural element, causing concentrations of high stresses in the remaining of contact's region. This kind of problem can be defined as unilateral contact problem and it was initially treated as a minimization problem without constraint or by using techniques of mathematical optimization. Recently, numerical approximations involving buckling and post-buckling of beams and plates under unilateral contact constraints imposed by elastic foundation appear in several papers. However, little is known on the behavior of arches submitted to unilateral contact constraints. So, the main objective of the paper is to present a geometrically nonlinear analysis of arches submitted to unilateral contact constraints, highlighting the influence of the stiffness of the geological medium on the buckling and equilibrium of these structural systems. The contact problem is solved as a linear complementary problem using Lemke's algorithm. Newton's iterations coupled with path-following techniques are employed to obtain the new contact forces and the nonlinear equilibrium configuration. The displacement field is update by using a Lagrangian formulation does not taking into account the influence of friction in the contact area. A geometrically nonlinear beam-column element is used to model the slender structure while a bed of spring that exhibits a sign-dependent force-displacement relationship is used to model the geological medium. The numerical solution strategy is verified by analyzing the nonlinear behavior of an arch on an elastic foundation. The results also show that the proposed nonlinear formulation can be used successfully in many engineering problems with the unilateral contact constraints being imposed at the beginning or along the structure deformation process. In addition, the present work clarifies the influence of the foundation position and its stiffness on the nonlinear behavior and stability of curved structures. Therefore, engineers can use the proposed methodology for the design of several soil-structure interaction problems, in particular those involving non-coehise soils. Reference: Silveira, R.A.M., Nogueira, C.L. and Gonçalves, P.B. (2013) A numerical approach for equilibrium and stability analysis of slender arches and rings under contact constraints. *International Journal of Solids and Structures*. 50(1) 147-159.

Title: Estimating Cardiac Pressure Volume Loop Non-Invasively Using Computational Cardiac Models

Author(s): David Nordsletten, Myrianthi Hadjicharalambous, Liya Asner, *Kings College London*.

Medical imaging has emerged as a powerful non-invasive tool for assessing heart function and pathology. Capable of providing detailed information on anatomy, regional myocardial motion and blood flow, medical imaging provides detailed quantification of the kinematic behaviour of the heart through the cardiac cycle. Despite the advance made in diagnosis, linking kinematics to kinetics from medical images remains a challenge. Indeed, assessing kinetic quantities, such as the external work of the heart, typically require invasive measures such as pressure catheterization. Integration of imaging data with mathematical models has the strong potential to bridge the kinematic and kinetic gap. Computational cardiac models provide a construct for assessing myocardial strain, stress as well as metrics of cardiac work. Constructing and parameterizing patient-specific models based on clinically acquired data, computational mechanics provides a physics-based lens through which one can interpret the kinetics of the heart in both health and disease. While this approach holds promise, these models are challenging to parameterize and remain dependent on invasive measurements. In this presentation, we will present a novel modelling approach to patient-specific cardiac mechanical simulations that relies purely on non-invasive measures that can be readily gathered clinically. Ensuring minimal distortion from the data, we will present a modelling paradigm for data integration and boundary condition specification [2] using an energy-based regularization. We show that these conditions minimize artefacts stemming from imaging data, while retaining model accuracy. Core to the design of our model is practical identifiability and parameter uniqueness that is demonstrated for both active [3] and passive [2] model components strictly from non-invasive data. We then validate this method through an in silico pipeline, demonstrating accuracy and robustness of the method at parameterizing the myocardial tissue properties as well as intraventricular pressure. These techniques are subsequently applied to patient-specific data, illustrating the efficacy of this approach in vivo. [1] Hadjicharalambous, H. et al. Analysis of cardiac constitutive laws for parameter estimation using 3D tagged MRI. 10.1007/s10237-014-0638-9 [2] Asner, L. et al. STACOM Challenge: simulating left ventricular mechanics in the canine heart. Lecture Notes in Computer Science. 10.1007/978-3-319-14678-2_13 [3] Asner, L. et al. Estimation of passive and active properties in the human heart using 3D tagged MRI. In submission.

Title: Multi-Scale and Stochastic Modeling of Organic-Rich Shales: A Probabilistic Bottom-Up Approach

Author(s): Mohammad Mashhadian, Arash Noshadravan, Sara Abedi, *Texas A&M U.*

Oil and gas shale rocks are very complex, naturally occurring geomaterials which have gained significant attention in the past decades as a source of fossil fuel. The multiscale models are essential in predicting the mechanical properties at the macroscale based on the information on subscale structure of these materials. Recently a multiscale model has been developed by Abedi et al., 2015 [1] that aims at nano-chemomechanical characterization of organic-rich shales at micrometer and sub-micrometer length scales using coupled grid nano-indentation and energy dispersive x-ray spectroscopy (EDX) acquired at the same locations through clustering analysis. The measurements obtained from advanced experimental techniques such as coupled grid nanoindentation and energy dispersive x-ray spectroscopy are used to inform the physically-based multiscale model for organic rich shales consisting of three levels that spans from the scale of elementary building blocks (e.g. clay minerals in case of clay-dominated formations) of organic rich shales to the scale of the macroscopic inorganic/organic hard/soft inclusion composite. Thus far, this bottom-up approach has been utilized within a deterministic framework and as such does not account for the uncertainty in compositional and mechanical model parameters. However providing information in diverse and uncertain environment is a key factor in improving the robustness and reliability of the model predictions. This research focuses on incorporating uncertainty in modeling multiscale behavior of organic-rich shales by taking into account the uncertainty in main subscale features such as mineralogy mass percents, porosity, elastic and toughness properties of elementary particles. To that end, we use Maximum Entropy Principle (MaxEnt) to construct probabilistic descriptions of model inputs based on available information. The Monte Carlo simulation is then carried out to propagate the uncertainty across different scales and consequently construct probabilistic descriptions of macroscale properties. The methodological developments will be supported by a validation plan that incorporates both simulation and experimental test database. The combination of experimental characterization, micro-poromechanical modeling and uncertainty quantification and propagation proposed in this work is of great value in terms of improving the robustness in the prediction and identification of essential subsurface parameters in engineering scale, such as acoustic properties. [1] Abedi, S., Slim, M., Hofmann, R., Bryndzia, T., and Ulm, F.J. (2015) "Nano-Chemomechanical Signature of Organic-Rich Shales: A Coupled Indentation-EDX Analysis". under review.

Title: A High-Order Discontinuous Galerkin Solver for Unsteady Incompressible Turbulent Flows

Author(s): Gianmaria Noventa, Antonio Ghidoni, *U. Brescia*; Francesco Carlo Massa, Alessandro Colombo, Francesco Bassi, *U. Bergamo*.

Several variants of the Discontinuous Galerkin (DG) method are nowadays in widespread use in the CFD community. DG methods are Finite Element (FE) methods in which the discrete solution of the weak or variational form of the governing equations is approximated by means of polynomial functions, which are continuous within elements, but discontinuous at element interfaces. With respect to standard Finite Volume (FV) methods DG methods allow (i) to achieve high-order accuracy on possibly non-conforming grids with arbitrarily shaped elements, (ii) to locally adapt the polynomial approximation of the solution, and (iii) to devise very compact discretization schemes, well suited for implicit time discretization and for parallel implementation of the schemes. In this work we present the main features of the DG code MIGALE for the simulation of unsteady incompressible turbulent flows. A distinguishing feature of the method used in this work is the formulation of the inviscid interface numerical fluxes. It is based on the exact solution of the Riemann problem for the artificial compressibility perturbation of the locally 1D inviscid Euler equations and provides the necessary coupling between the discretized incompressibility constraint and the rest of the governing equations. Viscous terms are discretized according to the BR2 scheme. The turbulence model has been implemented in a non-standard way employing the variable $\omega \blacksquare = \ln \omega$ instead of ω and enforcing the fulfilment of realizability conditions for the modeled turbulent stresses. Two high-order time integration schemes were implemented with adaptive control of the time step: the fourth order/six stages explicit-single-diagonal-implicit Runge- Kutta scheme (ESDIRK46), the third order/three stages (ROS3PL) and fourth order/six stages (RODASP46) linearly implicit one-step Rosenbrock methods. A standard pseudo-compressibility method (the incompressibility constrain is relaxed by the compressibility parameter) and a dual-time stepping technique (DTS) were also implemented for the ESDIRK. The reliability, robustness and accuracy of the proposed implementation have been assessed by computing several unsteady test cases: (i) the laminar travelling waves on a doubly-periodic unit square, (iii) the turbulent flow around a NACA 0018 airfoil at different angles of attack and (iii) the turbulent flow around a vertical axis wind turbine.

Title: Initiation and Progression of Saccular Aneurysm Enlargement from Medical Image Data

Author(s): Fred Nugen, Thomas JR Hughes, *UT Austin*; Luca Dede', *EPFL*; Michael Borden, *North Carolina State U.*

We have developed a formulation of saccular aneurysm disease which is capable of growing saccular aneurysm geometries from patient-specific data. We use a rate-sensitive inelastic material which, when stressed beyond its pseudo-elastic limit, produces irreversible deformations. Our analysis is intended to quantify forces and stresses in unruptured intracranial saccular aneurysms, giving insight into the environments of aneurysms. As disease progresses, we compare the stresses with a postulated pseudo-elastic limit stress. Whether stress is lower or higher than the tissue's pseudo-elastic limit determines whether the modeled aneurysm is stable or enlarging. We use a Winkler foundation term to model support of external organs and distinguish healthy from diseased tissue. We have verified the theory on idealized and patient-specific artery geometries. Validation will be assessed from the model's ability to reproduce an observed aneurysm from a healthy configuration, and to predict future enlargement consistent with clinical experience. A future goal is to validate the theory on a large dataset. Perhaps most importantly, we draw parallels between biological presentations of aneurysms and the model's parameters. Proposed tissue measurements and experiments have been brought to clinicians and biomechanicians involved in early detection and treatment of aneurysms. The framework gives a common language of concepts--eg, collagen fiber, pseudo-elastic limit, and subclinical lesion--through which researchers in different fields, with different terminologies, can engage in an ongoing dialog: under the model, questions in medicine can be translated into equivalent questions in mathematics. If the model is valid, it provides necessary and sufficient conditions for aneurysm behavior that bridge fields. The work begins a formulation of a "shape norm" to provide risk measures directly from geometries. Good risk measures provide better treatment plans and reduce morbidity, mortality, and reoperative rates.

Title: Mesh-Free Nonordinary Peridynamic Bending

Author(s): James O'Grady, *UT Austin*.

The peridynamic theory of solid mechanics offers an integral based alternative to traditional continuum models based on partial differential equations. This formulation is particularly advantageous when applied to material failure problems that result in discontinuous displacement fields. This paper presents a meshfree implementation of a state-based peridynamic bending model based on the idea of rotational springs between pairs of peridynamic bonds. Energy-based analysis determines the properties of these bond pairs for a brittle material, resulting in a constitutive model that naturally gives rise to localized damage and crack propagation.

Title: Application of the Generalized Finite-Element Method to Crack Coalescence Simulations Utilizing Fixed, Coarse Finite-Element Meshes

Author(s): Patrick O'Hara, *UTC*; Piyush Gupta, Armando Duarte, *U. Illinois*.

Accurate high cycle fatigue life estimates are important in the civil, mechanical and aerospace design communities. In many material systems, fatigue crack formation begins with the propagation and coalescence of diffuse cracks, many of which may be present in the material from the time of manufacturing. In order to accurately perform high-fidelity failure analyses of such material systems, the ability to simulate the coalescence of discrete crack surfaces is a requirement. This problem has recently been under investigation with the use of the generalized finite element method (GFEM) [1] which offers the advantage that the crack surfaces need not fit the finite element mesh. This alleviates the cumbersome meshing requirement, and likely user-intervention throughout the course of a simulation. While the GFEM offers gains in computational efficiency, a highly adapted mesh is still used in order to maintain solution accuracy. In order to improve computational efficiency, as well as to extend the range of applicability of GFEM-type approaches, a multi-scale version of the GFEM, termed the generalized finite element method with global-local enrichment functions (GFEMgl) [2] has also been under development. The GFEMgl is based on the use of specifically-tailored enrichment functions computed on-the-fly with the aid of a fine-scale boundary value problem defined in the neighborhood of a crack. In this manner, enrichment functions need not be known a priori, and the methodology is able to resolve localized features which themselves are smaller than the elements used in the simulation. This work focuses on an extension of the GFEMgl to address crack interaction and coalescence analyses. The numerical examples presented illustrate the potential of the method to utilize computational elements which are potentially larger than the coalescing crack surfaces, thus yielding computationally efficient crack coalescence simulations. References [1] J. Garzon, P. O'Hara, C.A. Duarte, and W. Buttlar. Improvements of explicit crack surface representation and update within the generalized finite element method with application to three-dimensional crack coalescence. *International Journal for Numerical Methods in Engineering*, 97:231–273, 2014. doi: 10.1002/nme.4573. [2] D.-J. Kim, J.P. Pereira, and C.A. Duarte. Analysis of three-dimensional fracture mechanics problems: A two-scale approach using coarse generalized FEM meshes. *International Journal for Numerical Methods in Engineering*, 81(3):335–365, 2010. doi: 10.1002/nme.2690.

Title: Coupling of 3D and 1D Transport Models to Predict Particle Deposition in the Pulmonary Airways

Author(s): Jessica M. Oakes, Shawn C. Shadden, *UC Berkeley*; Céline Grandmont, Irene E. Vignon-Clementel, *INRIA* .

Coupling of 3D and 1D Transport Models to Predict Particle Deposition in the Pulmonary Airways Jessica M. Oakes^{1,2,3}, Céline Grandmont^{2,3}, Shawn C. Shadden¹, Irene E. Vignon-Clementel^{2,3} (1) University of California Berkeley, Department of Mechanical Engineering, Berkeley, CA, USA (2) INRIA Paris-Rocquencourt, FRANCE (3) Laboratoire Jacques-Louis Lions, Sorbonne Université, UPMC Univ Paris 6, FRANCE Recent advances in computational resources have enabled sophisticated airflow and particle transport simulations in the pulmonary airways, however it is currently unfeasible to solve for airflow and transport for all length scales of the lung. Furthermore, while there has been significant focus on predicting particle transport during inspiration [1] there is limited knowledge on particle deposition during expiration. In this paper we present a new framework that couples 3D and 1D flow and transport models, enabling predictions of whole lung particle deposition throughout respiration. In the 3D domain the particle trajectory is determined by solving a reduced form of the Maxey-Riley equation by Lagrangian methods [1]. Throughout inhalation, particles either exit downstream of the conducting airways or deposit on the airway wall. Once particles exit the 3D model their concentration is passed to the single-path 1D model [2]. The 1D model incorporates lobar-specific dimensions that expand and contract throughout respiration and a loss term to model particle deposition due to gravitational, inertial and diffusive forces. Lobar deposition fractions agreed well with in vivo experimental data in healthy rat lungs [3] for particles with mass median aerodynamic diameter (MMAD) of 1.2 microns. Three times more particles deposited in the 3D conducting airways during exhalation than during inhalation. This enhanced deposition is caused by the slow flow rate during the last 0.1 seconds of exhalation, allowing time for the particles to settle. This framework may be applied in future studies to determine lung burden in diseased lungs (e.g. patients with chronic obstructive pulmonary disorder (COPD) or asthma). This work was supported by an INRIA Postdoctoral Research Grant and an University of California Presidential Postdoctoral Fellowship. [1] Oakes et al. Airflow and particle deposition in health and emphysema: from in vivo to in silico animal experiments. *Annals of Biomedical Engineering*, 2014, 44: 899-914. [2] Taulbee and Yu. A theory of aerosol deposition in the human respiratory tract. *Journal of Applied Physiology*. 1975, 38: 77-85. [3] Oakes et al. MRI-based measurements of aerosol deposition in the lung of healthy and elastase-treated rats. *Journal of Applied Physiology*. 2014, 116: 1561-1568.

Title: A Three-Dimensional Remeshed Hybrid Smooth Particle-Mesh Method for the Simulation of Compressible Turbulent Flow

Author(s): Anas Obeidat, *U. Luxembourg.*

We present a remeshed hybrid smooth particle-mesh method (hr-SPH) for the simulation of three-dimensional compressible turbulent flow. The proposed scheme is based on the remeshed smoothed particle method introduced by Chaniotis et al. [1] and Chatelain et al. [2]. In hr-SPH a mesh is introduced for efficient calculation of the pressure gradient, and laminar and turbulent diffusion. In addition, the mesh is used to remesh the particles to ensure a regular particle distribution and convergence of the method. The particles are remeshed (periodically reinitialised) onto uniform grid using a high order interpolation to overcome the particle clustering or distortion. The mass and the impulse of the particles are interpolated onto the mesh, where the rate of change and velocity are computed. These are used to update the velocity and the position of the particles. The method enjoys both, the Lagrangian properties of the SPH along with the efficiency of the finite difference computation. The method is capable of providing quality simulations while maintaining its robustness and adaptivity. Direct numerical simulations (DNS), along with Smagorinsky [3] model are applied in this study. To validate the method we perform a series of benchmarks, including: Two- and three-dimensional Taylor-Green flow [4]. Thin double shear layer [5]. Three-dimensional isotropic turbulence. we were able to resolve the double thin shear layer without producing the spurious vortical structure with a coarser mesh than what other studies suggested. And finally, the hrSPH method resolved the three-dimensional isotropic turbulence flow with high Reynolds number on a coarse mesh using Smagorinsky model. [1] Chaniotis A. K., Poulikakos D., and Koumoutsakos P. Remeshed smoothed particle hydrodynamics for the simulation of viscous and heat conducting flows. *J. Comput. Phys.*, 182(1):67–90, 2002. [2] Chatelain P., Cottet G.-H., and Koumoutsakos P. PMH: Particle-mesh hydrodynamics. *Int. J. Mod. Phys. C*, 18(4):610–618, 2007. [3] Smagorinsky J. General circulation experiments with the primitive equations, part I: the basic experiment. *Monthly Weather Rev.*, 91(3):99–164, 1963. [4] Taylor G. I. and Green A. E. Mechanism of the Production of Small Eddies from large ones. *Proc. R. Soc. Lond.*, 158(893):499–521, 1937. [5] Minion M. L. and Brown D. L. Performance of under-resolved two- dimensional incompressible flow simulations, II. *J. Comput. Phys.*, 138:734–765, 1997.

Title: Influence of Structural Solutions on Strength Behaviour and Instability of Straight Bars

Author(s): J.B. Obrebski, *Warsaw U. Tech.* .

In the paper will be shown comparative results of some series of calculated tasks explaining influence of structural solutions on instability of straight bars. There, will be compared for almost identical bars, this time, with identical length, but for example with changed one of the following elements of tasks: 1. combined external loadings with three components e.g.: two bending moments and longitudinal force (compressing or tensioning), two continuous transversal loadings and longitudinal force (as above), etc., eccentric longitudinal force combined with other loadings mentioned above, etc. 2. Bar boundary conditions by identical other elements of the task. 3. Type of cross-section. 4. Thin-walled or full cross-section, homogenous or composite - built of some different materials. 5. Symmetry, bisymmetry of cross-section giving different positions of shearing centre of the cross-section. Any combination of above elements of the task, etc. Moreover, or rather first of all, will be shown for instability problems instability critical surfaces depending on all above elements of the task, embracing safe "areas" and combination of listed above parameters giving critical – unstable state of structure. All above mentioned examples are based on own theory [1] and on defined by present author uniform criterion for instability – when main determinant of analyzed equations is equal zero. The present paper provides results of the following investigations too. 1. Numerical and experimental verification of own very efficient theory for mechanical analysis of straight bars behaviour. 2. Strength analysis of bars with homogenous or composite, thin walled or full, symmetrical, bisymmetrical, unsymmetrical cross-sections. 3. Critical stability curve called "izostaba line" which together with critical ultimate surfaces is efficient tools for safe designing of the bars. 4. Good convergence of theoretical results for statics and stability of bars with experiments, own and specially executed tests made by other researchers for industrial practical designing. References [1] J.B. Obrebski: Thin-Walled Elastic Straight Bars (In Polish – Cienkoscienne Sprezyste Pretly Proste. Publishing House of Warsaw University of Technology (OWPW), Warsaw, 1991, 1997.

Title: A Shear-Deformable, Rotation-Free Isogeometric Shell Formulation

Author(s): Bastian Oesterle, Ekkehard Ramm, Manfred Bischoff, *U. Stuttgart*.

Isogeometric Analyses using NURBS functions enable a smooth surface description with higher inter-element continuity which opens up new possibilities in the analysis of thin-walled structures. An important advantage is the straightforward implementation of classical theories, which require C1-continuity, e. g. Kirchhoff-Love shell formulations, as demonstrated in [1]. Based on these simplest models, also shear deformable theories, like Reissner-Mindlin shell formulations, can be formulated in an elegant way. In [2] a hierarchic set of isogeometric shell finite elements is developed, avoiding shear locking within the framework of a pure displacement formulation. Further investigations lead to a shear-deformable, rotation-free isogeometric shell formulation naturally free from shear locking and with improved quality of stress resultants. The underlying idea is the split of displacements into bending and shear parts, which can also be observed for beams in [3]. A current challenge is the removal of membrane locking within a purely displacement concept. References [1] J. Kiendl, K.-U. Bletzinger, J. Linhard, R. Wüchner. Isogeometric shell analysis with Kirchhoff-Love elements. *Computer Methods in Applied Mechanics and Engineering*, 198:3902–3914, 2009. [2] R. Echter, B. Oesterle, M. Bischoff. A hierarchic family of isogeometric shell finite elements. *Computer Methods in Applied Mechanics and Engineering*, 254:170–180, 2013. [3] J. Kiendl, F. Auricchio, T.J.R. Hughes, A. Reali. Single-variable formulations and isogeometric discretizations for shear deformable beams. *Computer Methods in Applied Mechanics and Engineering*, 284:988–1004, 2015.

Title: Correlation Between Flow Field and Propulsive Efficiency of a Swimming Killifish

Author(s): Yoichi Ogata, Takayuki Azama, *Hiroshima U.*

The present paper discusses propulsive efficiency of a killifish with two motions, carangiform that a killifish takes in general and anguilliform as comparison. Flow fields generated by fish deformations are simulated by CIP method in combination with an immersed boundary method. It is found in our previous studies that time variations of swimming speed and fluid force of a small fish can be estimated like a free fall model with low Reynolds number, and fluid force can be separated into thrust and viscous drag. Flow fields visualized using second and third invariants have also shown that a fish with carangiform can be accelerated faster and efficiency also larger by larger thrust due to the strong transverse vortex in the wake of the fish, but also spends larger swimming power due to larger drag than a fish with anguilliform.

Title: A Scaled-BDD Preconditioner for the Schur Complement Equation

Author(s): Masao Ogino, *Nagoya U.*

For many of actual problems in science and engineering fields, there should be modeled with multi-materials and large-scale unstructured mesh. The Domain Decomposition Method (DDM) based on the iterative methods is well-known as an effective parallel finite element method, however, solving such problems will suffer from slow convergence or no convergence. In order to achieve high performance in both convergence rate and parallel efficiency, it is necessary to apply an effective preconditioner for multi-materials. The Balancing Domain Decomposition (BDD) preconditioner is an effective preconditioner for its very fast convergence rate. However, in case of composition of very different materials for actual problems, the convergence rate of the BDD is also shown to be worse. Some studies extended the BDD preconditioner to such problems with jumps in coefficients, but these are not suitable for complex shape model and parallel computing. In this study, to accelerate convergence of the BDD preconditioner for multi-materials, a Scaled-BDD is proposed and some numerical examples are shown.

Title: Stochastic-Dynamic Earthquake Models and Tsunami Generation

Author(s): David Oglesby, *UC Riverside*; Eric Geist, *US Geological Survey*.

Dynamic earthquake rupture models are now understood to provide physically plausible faulting scenarios for ground motion estimation, but their use in tsunami hazard analysis is in its infancy. Typical tsunami generation methods rely on kinematic or dislocation models of the earthquake source, in which the earthquake magnitude, rupture path, and fault slip distribution are assumed a priori, typically based on models of prior earthquakes, aftershock distributions, and/or some sort of stochastic slip model. However, such models are not guaranteed to be consistent with any physically plausible faulting scenario, and may span a range of parameter space far outside what is physically realistic. In contrast, in dynamic models the earthquake rupture and slip process (including the final size of the earthquake, the spatiotemporal evolution of slip, and the rupture path on complex fault geometry) are calculated results of the models. Utilizing the finite element method, a self-affine stochastic stress field, and a shallow-water hydrodynamic code, we calculate a suite of dynamic earthquake models and near-source tsunamis from a branched megathrust/splay fault system (i.e., where one of the earth's tectonic plates is subducted under another) that is motivated by the geometry in the Nankai region of Japan. Different stress realizations produce different spatial patterns of slip, including different partitioning of slip between the megathrust (the main plate boundary fault) and splay (steeper intersecting fault) segments. In particular, we find that the state of random stress near the megathrust/splay intersection has a controlling influence on a bimodal distribution of ruptures—ones that rupture primarily on the steeper splay, and ones that rupture primarily on the more shallow-dipping megathrust. Because the partitioning of slip between fault segments has a first-order effect on the surface deformation and tsunami generation, the modeled near-source tsunamis are also highly variable, with a rather bimodal distribution as well. We will discuss the implications of these results for both seismic and tsunami hazard estimations.

Title: Modal Analysis of Vibrations of Liquids Coupled with Structures

Author(s): Roger Ohayon, *CNAM* ; Jean-Sebastien Schotte, *ONERA* .

We review the basic equations and corresponding variational formulations of the linearized vibrations of a liquid with a free surface contained in an elastic structure. In hydroelastic standard situations, the liquid is considered as incompressible, gravity effects being taken into account through appropriate fluid-structure interface operator referred as elastogravity operator using a scalar field (pressure and/or displacement potential fields for the fluid). Compressibility effects for the fluid can then be introduced, using a Lighthill model for the basic equations of compressibility/gravity interactions, the fluid irrotationnality condition being replaced, in general, by a plane-irrotationnality equation.

Title: Interaction Integral Method for Arbitrary Shaped 3-D Cracks and its Application in Crack Propagation Problems

Author(s): Hiroshi Okada, Yuki Wakashima, Hiroshi Kawai, *Tokyo U. Science.*

In this research, we have been developing a fracture/crack propagation analysis system for damaged structures. The system can fully automate the crack propagation analysis. The analysis system is based on the Finite Element Method (FEM) to perform the solid mechanics analysis and the Delaunay tessellation technique to generate the finite element mesh. The stress intensity factors that characterize the direction and rate of crack propagation are evaluated by the interaction integral method for the quadratic tetrahedral finite element. Mesh generation processes are automated by using the Delaunay tessellation technique. The interaction integral method for the quadratic tetrahedral element that has been developed by the authors (Daimon and Okada [1]) is extended so that it can accurately evaluate the stress intensity factors even when the finite element mesh is arranged in a totally random manner and when the crack has curvatures and kinks. The method can be applied to plural crack problems in which two neighboring cracks are very close to each other. The virtual crack propagation vector for the domain integral method is set to be zero at the locations where additional surface integral term and singularities due to crack kinking arise. When the integral domain include the neighboring crack, the virtual crack extension vector is set to be zero on the surface of the neighboring crack. The same thought is seen in Okada and Ohata [2]. It is noted that by the use of the correction term introduced by Daimon and Okada [1], the stress intensity factors can be accurately even when an unstructured mesh is adopted in the vicinity of the crack. In the presentation, we will discuss about the formulation of proposed interaction integral scheme and crack propagation analysis system. Then, some numerical demonstration problems are presented. [1] R. Daimon and H. Okada, "Mixed-mode stress intensity factor evaluation by interaction integral method for quadratic tetrahedral finite element with correction terms", *Engrng Fract. Mech.*, 115, 22–42, (2014). [2] H. Okada and S. Ohata, "Three-dimensional J-integral evaluation for cracks with arbitrary curvatures and kinks based on domain integral method for quadratic tetrahedral finite element", *Engrng Fract. Mech.*, 109, 58–77, (2013).

Title: Strong Coupled Analysis by Multi-Material Eulerian Hydrocode

Author(s): Shigenobu Okazawa, Hirofumi Ueda, Toru Hamasaki, *Hiroshima U.*

This paper describes computational method for multi-material Eulerian hydrocode for large deformation solid-fluid coupled problems. We solve this problem in unstructured mesh using stabilized finite element method. In the Eulerian formulation for the path-dependent solid deformation, stress and any path-dependent variables must be advected. Although the path-dependent variables are defined on integration point in mesh, the stabilized finite element method can advect variables in only node. The present paper approximates variables on node using information in mesh, and advects the variables on node. We test the present approach in representative computational examples including hyperelasticity, elastoplasticity and viscosity.

Title: Sensitivity Analysis and Model Uncertainty Quantification for RANS Models of Separated Flows

Author(s): Todd Oliver, Vikram Garg, Robert Moser, *UT Austin*.

In this talk we examine the sensitivity of aerodynamic quantities of interest (QoIs) to turbulence modeling errors for separated or nearly separated flows like the flow over an airfoil or wing near stall. In the engineering analysis of such flows, it is common to use the Reynolds-averaged Navier-Stokes equations coupled with an eddy-viscosity-based turbulence model. Such models are attractive because, relative to higher-fidelity modeling approaches, they are computationally inexpensive. However, these models require that the Reynolds stress tensor---which quantifies the effects turbulence on the mean flow field---be closed in terms of the mean flow. Such closures are typically developed based on clearly stated but questionable modeling assumptions. These assumptions are often reasonable for statistically two-dimensional attached flows, and RANS models often perform quite well for such flows. However, in separated flows, the underlying modeling assumptions tend to break down. Moreover, it is well-known that smooth-wall separation locations can be sensitive to characteristics of the upstream boundary layer. Thus, in addition to modeling errors introduced in the separated region itself, significant errors in QoIs sensitive to separation location may be introduced by seemingly small errors in the Reynolds stress in the upstream boundary layer. Thus, in this talk, we will explore the sensitivity of aerodynamic QoIs like lift, drag, and pitching moments to errors in the Reynolds stress for mildly separated flows, such as a typical airfoil flow nearing the stall angle of attack. This exploration will take advantage of techniques from both local sensitivity analysis and uncertainty quantification. For instance, using adjoint solutions, we will compute the sensitivity of the QoIs to perturbations in the Reynolds stress field. This analysis will give insight into where in space the Reynolds stress is most influential to the QoIs and allow linearized forward propagation of small modeling errors to the QoIs. To investigate larger errors, we will develop simple random field models to represent possible errors in the Reynolds stress and propagate these errors forward to the QoIs.

Title: A Consistent Energy-Based Atomistic-to-Continuum Coupling Method for Multilattices

Author(s): Derek Olson, Mitchell Luskin, *U. Minnesota*; Alexander Shapeev, *Skoltech*.

Significant progress has been made in the development and analysis of atomistic-to-continuum (AtC) coupling methods for crystalline materials described by a Bravais lattice in one and two dimensions, but few results are known for multilattices. We present a new AtC method suitable for modeling multilattices in one and two dimensions when the atoms interact via an empirical pair potential. This method is based on the consistent energy-based method of Shapeev (2011) and is constructed by converting a bond-based continuum energy into a volume-based continuum energy. The volume-based continuum energy is predicated upon the definition of a type of quadrature point for each triangle, and these points can be efficiently pre-computed. We show the method satisfies a patch test criterion and estimate the consistency error made in the approximation. We hypothesize additional assumptions under which the method is stable and provide subsequent error estimates.

Title: Early Detection of Breast Cancer Through an Inverse Problem Approach to Stiffness Mapping: Preliminary Results from Tissue Phantom Experiments

Author(s): Lorraine Olson, Robert Throne, Adam Nolte, Allison Crump, Wanli He, Michael Jones, Caitlin Douglas, Matthew Conrad, Emily Cottingham, *Rose-Hulman Inst. Tech.*

Early detection of breast cancer will continue to be crucial in improving patient survival rates. Manual breast exams and mammograms are currently the most widely used techniques for early detection. Manual breast exams rely heuristically on the significant stiffness (elastic modulus) difference between cancerous tissue and healthy tissue. We are working to systematize this approach by developing an inverse technique which is capable of inferring the stiffness throughout the breast tissue based solely on surface displacement measurements. Finite element methods are used to model the tissue response for the forward problem-- solving for the surface tissue displacements for a given indentation pattern. A genetic algorithm is used to solve the inverse problem-- given the measured surface displacements, what is the distribution of tissue stiffness within the breast? Results from three-dimensional simulations have been promising. Healthy tissue was modeled with an elastic modulus of 3 kPa and cancerous "tumors" at 20 kPa. We tested seven cases with tumors and one tumor-free case, employing 50 trials of each. For these simulations the "measured results" were generated with healthy tissue properties that varied randomly in the range 3 ± 1 kPa and cancerous tissues at 20 ± 4 kPa, with 20 dB noise. Using our standard fitness function we found only 4 false positives and 1 false negative out of the 400 trials. Tissue phantom experiments are the next stage for validation and improvement of the method. A gelatin phantom is cast in a spherical mold, with or without tumors. The stiffness of the phantom is controlled primarily by adjusting the gelatin mass fraction. The phantom is indented in a known pattern with a tool manipulated by a Scorbot ER-4u (Intelitek) robot. Surface coordinates are measured before and after indentation with an Aramis Optical Deformation Analysis System 5M (GOM) and normal surface displacements are calculated from that data. The initial coordinates are used to create a finite element model for the forward problem. The finite element model and displacement measurements are used as input to the genetic algorithm. Preliminary results for the method when phantoms are cast with and without tumors will be presented. We wish to thank Michael Insana (University of Illinois) and Scott Small and Renee Rogge (Rose-Hulman Institute of Technology) for their advice and support. This material is based upon work funded by the National Science Foundation under Grant No. ECCS-1306808, and used the Extreme Science and Engineering Discovery Environment (XSEDE, NSF grant OCI-1053575.)

Title: Spacetime Discontinuous Galerkin Finite Element Method and an Interfacial Damage Model for Hydraulic and Compressive Fracture Simulations

Author(s): Omid Omid, Reza Abedi, *U. Tennessee Space Inst.*; Saeid Enayatpour, *UT Austin*; Ian McNamara, Robert Haber, *U. Illinois, Urbana-Champaign*.

Rocks are heterogeneous at different scales. At small grain scale, they are characterized by the presence of microcracks and granular microstructures. In fact, a rock material contains a large number of randomly oriented zones of potential failure in the form of grain boundaries. At large mass scale, they are described by the presence of different rock types, faults and weak features such as fracture networks. These inhomogeneities affect the mechanical response of rocks. In this paper, an interfacial damage model implemented in a Spacetime Discontinuous Galerkin (SDG) framework is employed to numerically explore the mechanisms underlying rock fracture and contact under dynamic loading. Three main components of our model are: 1) Modeling complicated fracture patterns: Due to the existence of natural fracture networks in rocks, robust numerical methods must be employed for fracture modeling. We use the SDG method's powerful adaptive operations to directly track crack propagation directions with element boundaries. Consequently, unlike eXtended Finite Element Methods (X-FEMs) no basis function enrichments are required inside elements; 2) Contact-fracture mode transitions: Since rocks are often under large compressive loads they experience frequent transitions between various contact modes. We present a seamless framework to transition from the dynamically-consistent contact modes to tensile/shear crack propagation mode; 3) Material inhomogeneities: We employ two approaches to model rock inhomogeneities. First, fractures with random size, location and orientation model natural pre-existing crack-like defects. Second, a probabilistic nucleation approach is used to model generation of new cracks due to excessive loads. Rocks exhibit two principal responses to stresses being exerted on them, one in tensile mode and another in shear mode. We present two applications where one of these modes is the dominant mechanism of crack propagation. In the first example, hydraulic fracturing, we utilize the adaptive meshing schemes of the SDG method to track new crack surfaces generated by hydraulic pressure on the fracture surfaces. We performed a sensitivity analysis of input variables such as the magnitude of in-situ stress components, number and orientation of induced fractures to demonstrate the effectiveness of our approach in resolving hydraulic fracturing in shale plays. For the second example, a rock specimen with randomly-distributed defects is simulated under dynamic compression. While being mainly in compressive mode, the high shear stresses induced from the impact cause the nucleation of new cracks and propagation of pre-existing microcracks. We will discuss how the initial distribution of defects affects macroscopic fracture patterns.

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Title: Cellular Scale Physiological Flow: Active Swimming Sperm Cells and Passive Flowing Red Blood Cells

Author(s): Toshihiro Omori, *Toshoku U.*; Takuji Ishikawa, Yohsuke Imai, Takami Yamaguchi, *Tohoku U.*.

In this study, we investigated cellular scale physiological flow using a boundary element method. Especially, we analyzed motion and deformation of red blood cells in blood flow to understand how they affect macroscopic blood rheology and mass transport. We also investigated motions of motile sperm cell near plane wall. We find that the sperm cell, in shear flow, tends to turn to upstream and swims against fluid flow. This result indicates that rheotaxis of sperm cells might be explained by fluid dynamics.

Title: Application of Preconditioned Iterative Methods in Selective Smoothed Finite Element Methods with Tetrahedral Elements for Nearly Incompressible Materials

Author(s): Yuki Onishi, *Tokyo Inst. Tech.*

Smoothed finite element methods (S-FEMs) are promising for efficient finite element formulations in solid mechanics problems. The selective S-FEMs [1] are known to have an especially unique advantage: locking-free even with tetrahedral elements for nearly incompressible materials. In contrast to hybrid or mixed finite element methods, S-FEMs use only nodal displacement DOFs and do not necessitate any additional unknown such as pressure. Therefore, the S-FEM's matrix in the equation to solve can be explicitly built without Lagrange multiplier nor static condensation, which enables the simple application of fully preconditioned iterative methods. Solving the S-FEM's matrix equation for nearly incompressible materials with iterative methods is an important issue for the parallel computing of large-scale problems. In this study, the capability of preconditioned iterative methods in selective ES/NS-FEM with tetrahedral elements (ES/NS-FEM-T4) is investigated. The generalized minimal residual (GMRES) method with the algebraic multigrid (AMG) preconditioner (AMG-GMRES) is adopted as the preconditioned iterative method. As is the case in other FEMs, the condition number of the ES/NS-FEM-T4's matrix becomes bigger and bigger as the Poisson's ratio of the material approaches to 0.5. However, increase in the number of cycles of AMG preconditioning improves the condition number for GMRES and helps its convergence to some extent. It is also remarkable that the ES/NS-FEM-T4's matrix generally satisfies the extended definition of positive-definite for non-symmetric matrices. Some examples of analysis reveals that AMG-GMRES works well in ES/NS-FEM-T4 even in the case of large deformation of nearly incompressible materials. [1] Y. Onishi et. al, "A locking-free selective smoothed finite element method using tetrahedral and triangular elements with adaptive mesh rezoning for large deformation problems", *Int. J. Numer. Meth. Engng*, 2014; 99: 354-371.

Title: Crystal Level-Phase Transformation with a Dislocation Based Strength Model

Author(s): Saul Opie, K. Krishnan, S. Gautam, A. Brown, P. Peralta, *Arizona State U.*; E. Loomis, *Los Alamos Nat'l. Lab.*

Pressure-induced martensitic phase transformations are common in many shock loaded materials, particularly metals. Steady shock waves with phase transformations are qualitatively captured well at the macroscopic level by combining a simple isotropic strength model with an Equation of State (EOS) that accurately reproduces the equilibrium phase surface. However important and experimentally observable details such as the kinetics of the phase change, orientation dependence, and shear strain influence are all largely unaddressed with this approach. To satisfactorily explain these observations a physically based microstructure model is needed. Alternatively, experiments with phase transformations can be used as another indirect verification tool for high strain rate dislocation based strength models. The work presented here builds upon the crystal level phase transformation framework suggested by [1], which is able to capture the iron alpha to epsilon texture evolution observed in diamond anvil experiments well. Modifications include a thermoelastic framework similar to [2] and a recent dislocation based strength model [3] with appropriate modification for lower symmetry crystals. As in [1] dislocation density is passed with transforming mass fractions. Preliminary computational results will be presented and compared to experimental phase transformation kinetics (e.g. [4]).

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Title: A Computational Framework for Polyconvex Large Strain Electromechanics Applications

Author(s): Rogelio Ortigosa, Antonio J. Gil, Javier Bonet, *Swansea U.*

The present work focusses on the simulation of Electro Active Materials (EAMs). A wide range of materials can be classified under that denomination. Among those, piezoelectric ceramics, piezoelectric polymers and more recently, Dielectric Elastomers (DE) have been applied as actuation and energy harvesting devices in an overwhelming variety of industrial applications. For instance, these materials have been recently used for morphing wing control in unmanned aerial vehicles and for the precise shape control of scale space antennas. In most applications, these materials appear in the form of thin patches mounted directly to a relatively thin structure. Therefore, suitable beam/shell models can be applied for their reliable numerical simulation. We present a variational formulation for beam/shells which relies on a Taylor series expansion of displacements and electric potential across the section of the beam. Unlike classical beam theories, where the definition of engineering strain measures arise, the present approach represents an extension of the continuum degenerate beam formulation presented in reference [1] to the more general case of electro-mechanics. The current formulation is applicable to large deformation scenarios, where appropriate constitutive restrictions are crucial. In particular, our constitutive models are defined in terms of an internal energy function based on a polyconvex combination of both strain and electric variables [2]. Very remarkably, these materials have been applied in Microelectromechanical Systems (MEMS), either for sensing, actuation or transduction purposes. High accuracy is needed in the simulation of this type of applications. Hence, the influence of Maxwell vacuum stresses must not be disregarded. We present an approach in which the influence of the surrounding vacuum is included in a surface integral through the Boundary Element Method [3]. We propose a modified version of the resulting boundary integral in order to remove possible singularities of the integrands containing the fundamental solution of the associated Laplace's equation. References: [1] R. Ortigosa, A.J. Gil, J. Bonet. A computational framework for polyconvex large strain elasticity for geometrically exact beam theory, under review. [2] A.J. Gil, R. Ortigosa, J. Bonet. A computational framework for polyconvex large strain electromechanics, under review. [3] D. K. Vu and P. Steinmann. On 3-D coupled BEM-FEM simulation of nonlinear electro-elastostatics. Computational Methods in Applied Mechanics and Engineering, 58, pp. 79-116, 1986.

Title: High-Order Nonlocal Multiscale Homogenization Model for Analysis of Wave Propagation in Composite Materials

Author(s): Tong Hui, Ruize Hu, Caglar Oskay, *Vanderbilt U.*

We present the formulation and implementation of the high order nonlocal multiscale homogenization model for analysis of wave propagation in viscoelastic and elastic composite materials subjected to dynamic loading condition. The proposed model is derived based on the asymptotic homogenization method with multiple spatial scales. Asymptotic expansions of the associated response fields up to sixth order are employed to capture wave dispersion in the presence of non-uniform density and non-uniform moduli within the material microstructure. Hybrid Laplace Transform/Finite Element Method is employed to solve for displacement field in Laplace domain therefore the imaginary part of solution is retained, which enables this model to capture the wave attenuation effect within the band gap. Response field in time domain is obtained by applying discrete inverse Laplace transform method. By eliminating the temporal and microscopic coordinate dependency, the proposed model has demonstrated high level of computational efficiency. The key contributions of this work are: (1) wave dispersion in elastic composite material and viscoelastic composite material is accurately predicted under a wide range of loading and material parameters. (2) energy dissipation in viscoelastic material is well captured by taking account linear viscoelastic constitutive relationship using a proportionality law. (3) the onset, width and wave attenuation behavior of band gap is accurately captured accounting for microstructural length, density and elastic modulus only, without introducing any parameters that need to be further determined. Numerical examples of wave propagation in elastic and viscoelastic composite materials will be presented. The wave dispersion and dissipation characteristics in both layered and particulate composite materials will be discussed. The onset, width and wave attenuation behavior of band gap will be illustrated.

Title: Dislocation Dynamics via the Extended Finite-Element Method

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

As the Volterra construction of a dislocation is a prescribed discontinuity along an internal surface within a body, the extended finite element method provides a straightforward means of modeling the elastic fields generated by dislocations. Since the discontinuity of the displacement field across a slip plane is fixed to specific crystallographic lattice translation vectors, i.e. Burgers vector, the effect of the dislocation enrichment functions on the discretized finite element equations appears on the right hand side as an additional nodal force. In this talk, it will be shown that the configurational forces relating the strain energy of the body to the position of dislocations can be computed in a more efficient manner than for fracture simulations by exploiting the fixed nature of the discontinuity. Examples of dislocation propagation near free surfaces and interfaces will show the applicability of the method to modeling realistic materials.

Title: A Piecewise Model Order Reduction Method for the Simulation of the Nonlinear Behavior of Wire Ropes

Author(s): Nerea Otano Aramendi, *Ecole Centrale Paris; IKERLAN*; Damien Durville, *Ecole Centrale Paris*; David Neron, *L.M.T CACHAN*; Hodei Usabiaga, *IKERLAN*; Mikel Urchegui, *ORONA*.

Multi-strand wire ropes used in elevators have a two-level structure in which elementary wires are first arranged into strands, which are then assembled to form the rope. Simulating the mechanical behavior of such structures when passing over the sheaves of elevators is required to assess contact-friction interactions taking place between wires. A finite element simulation code, based on an implicit solver [1], can be employed to perform such simulations. However, due to the different nonlinearities considered in the problem (finite strains, contact and friction), and to the large number of wires involved in such ropes (typically between 100 and 200), the simulations are computationally too expensive if we want to consider a rope whose length is of the order of few diameters of the sheave. The aim of this work is to propose a Model Order Reduction technique, based on a Proper Orthogonal Decomposition, to reduce the computational cost of these simulations [2]. Taking advantage of the repetitive periodic structure of wire ropes, we propose a piecewise approximation of the solution using a local reduced-order basis. This basis is built off-line, using a singular value decomposition, from snapshots resulting from simulations of typical loading cases. First tests showed that only few modes were necessary to reproduce rather complex loading cases, such as the bending of a strand onto a sheave, with small errors. Since the identification of a reduced-order basis on the full considered rope would be too expensive, the reduced-order basis employed in the presented approach is identified only on a small representative elementary length of a strand. The considered rope is modeled as a series of elementary pieces, each of them being represented by the modes of the elementary reduced-order basis. Special care is paid to the modeling of connections between these elementary modes, by keeping the degrees of freedom related to the junctions between pieces in the reduced problem, to allow displacement solutions on successive pieces to fit to each other. Details of the piecewise reduction method and results obtained on realistic loading cases will be presented. [1] D. Durville. Contact-friction modeling within elastic beam assemblies: an application to knot tightening. *Computational Mechanics*, 49(6):687–707, February 2012. [2] G. Berkooz, P. Holmes, J. Lumley, The proper orthogonal decomposition in the analysis of turbulent flows, *Ann. Rev. Fluid Mech.* 25 (1993) 539–575.

Title: Peridynamic Modelling of Underwater Shock Response of Marine Composite Structures

Author(s): Cagan Diyaroglu, Dennj De Meo, Erkan Oterkus, *U. Strathclyde*.

Composite structures have extensive area of practice in engineering disciplines. One of the application areas is to use them under extreme loading conditions. However, our understanding of their behaviour at high strain rate, i.e. under shock loading conditions, is rather limited as opposed to under static conditions. As a result of this, current designs of composite structures are very conservative for high velocity impact loadings which significantly reduces the weight saving advantage of composite materials. In order to improve our understanding, experimental studies are essential, but they can be prohibitively costly. On the other hand, computer simulations can be a good alternative of experimental tests. Hence, the main objective of this study is to investigate underwater shock response of composite structures by using a new computational technique called Peridynamics. Peridynamics is a state-of-the-art-technique which is especially promising tool for failure analysis of structures. It is basically reformulation of continuum mechanics and its equation of motion is in the form of an integro-differential equation rather than a partial differential equation as in the classical continuum mechanics. This feature allows continuous usage of equations regardless of discontinuities such as cracks. In this study, the developed approach is used to predict the failure modes in marine composite structures as a result of underwater shock phenomenon. The evaluated results are validated by comparing against the available data in literature which will also demonstrate the capability of peridynamics for such complex problems.

Title: A Peridynamic Model for Hydraulic Fracture

Author(s): Hisanao Ouichi, Amit Katiyar, John Foster, Mukul Sharma, *UT Austin*.

We present a coupled nonlocal model based on peridynamic theory for the poromechanical deformation and failure of rocks targeting applications of hydraulic fracture. The model is capable of reproducing known analytic solutions to simple fracture geometries as the characteristic nonlocal length-scale vanishes; however, the nonlocal nature of the formulation is particularly useful in regularizing (i.e., removing mesh dependence) cases of complex fracture propagation and coalescence of propagating hydraulic fractures with natural fractures. This presentation will show the model equations along with validation results for a series of test problems. Additionally, we show regularized large-scale simulations that exhibit sufficient complexity to demonstrate the utility of the model. This complexity includes the effects of heterogeneities in elastic, fracture, and fluid transport properties, as well as the effects of complex natural fracture networks on hydraulic fracture propagation.

Title: Auxiliary Subspace Error Estimation for Elliptic Problems

Author(s): Jeffrey Owall, *Portland State U.*

Auxiliary subspace error estimation may be viewed as a natural extension of traditional hierarchical basis error estimation, for which an approximate error function is computed in an auxiliary space. We consider families of Lagrange spaces (h, p or hp-versions) on simplicial meshes for second-order linear elliptic equations in any dimension, and describe suitable auxiliary spaces in which to approximate the error. Analyzing the approach as an h-method, we establish equivalence of error and error estimate (up to oscillation) in H^1 . Empirical evidence strongly suggests that equivalence holds as well for p and hp-methods, but a proof (or refutation) of this remains open. Mention will also be made of natural extensions to non-standard discretizations such as virtual element methods (VEM) and boundary-element-based finite elements (BEM-FEM). Much of the discussion is based on joint work with Michael Neilan (Univ. Pittsburgh) and Harri Hakula (Aalto Univ.).

Title: Parallel Mesh Optimization for Grid-Based Hex Meshes

Author(s): Steven Owen, *Sandia Nat'l. Lab.*.

A strategy for mesh smoothing is proposed for large scale unstructured hex meshes. Grid and octree-based meshing procedures have been shown to provide a successful automatic hex solution for arbitrary geometries. However, depending on geometric constraints, they can often suffer from poor quality elements at interface boundaries. We propose an effective smoothing solution that utilizes both shared and distributed memory to produce a usable FEA mesh for large-scale problems. A three-stage mesh improvement strategy is proposed: 1. Jacobi-based Laplacian smoothing utilizing MPI for distributed computing and OpenMP for shared memory is applied to all hexes. 2. For the remaining hex elements falling below a user defined quality threshold, Jacobi-based optimization is applied using a damping factor and a modified scaled Jacobian objective function. 3. For the difficult cases where steps 1 and 2 are not effective, a parallel coloring approach is used that identifies and isolates independent hex kernels and applies optimization to improve only the worst quality elements. This approach has the effect of progressively narrowing the scope of the smoothing procedures to focus only the poorest quality elements. We demonstrate its effectiveness through the results of a study of more than 50 CAD models where grid-based meshing is applied followed by the proposed smoothing strategy. A range of processor counts and mesh densities is also used, demonstrating parallel efficiency and consistency.

Title: Towards Understanding the Wave-Supported Gravity-Driven Mud Flows: Application of Direct Numerical Simulations

Author(s): Celalettin Ozdemir, *Louisiana State U.*

Direct Numerical Simulation (DNS) has become an invaluable and is sometimes the only tool that provides mechanistic explanations to near shore sediment transport processes and their accurate parameterization in larger scale ocean models. One particular example is the wave-supported gravity-driven fluid-mud flows (WSGDF) which have been observed to be one of the significant agents that shape the near shore morphology. WSGDF takes place in mild-sloped portions of a continental shelf where generation of turbidity currents is not possible. Fine riverine sediments that are deposited in the river mouth after a high river discharge are suspended due to turbulence in the wave boundary layer (WBL). Suspended sediments can be transported to significantly long distances offshore in the continental shelf under mild gravitational acceleration. WSGDF occurs when WBL is of transitional and intermittently turbulent nature. Therefore, DNS becomes the only numerical tool to accurately quantify and assess the flow in WBL and thereby fate of fine sediments. Furthermore, turbulence modulation due to sediment-induced stable density stratification plays a significant role in fine sediment transport which may even lead to laminarization in WBL and cannot be predicted by conventional Reynolds-averaged turbulence closure models. In this presentation, the effect of sediment-induced stable density stratification due to dense deposits in the river mouths, i.e., high mud concentrations, and that due to comparably larger sediment particles in the fluid-mud mixture, i.e., particles with higher settling velocity, on WBL through DNS shall be discussed. The results of these simulations, revealed four states of fluid-mud in a moderately energetic surface wave field: (i) fully turbulent regime where virtually no turbulence modulation is observed in the case of very dilute sediment concentration, (ii) slightly modified turbulent regime where a local and slight turbulence attenuation is observed, (iii) laminar regime with intermittent instability, and (iv) completely laminar regime due to strong particle-induced stable density stratification. These four regimes can explain the wave energy dissipation and transport of fine particles to long distances under mild gravitational acceleration.

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Title: Spectral Full-Field Deformation Modeling of 2-Phase Titanium Structures on a Spectrum of Alpha Fractions and Beta Morphologies

Author(s): Tugce Ozturk, Ross Cunningham, Robert Suter, Anthony Rollett, *Carnegie Mellon U.*; Reemu Pokharel, *Los Alamos Nat'l. Lab.*

The Fast Fourier Transform (FFT) based full field technique is used to model the mechanical deformation of polycrystalline materials in elastic, viscoplastic and elasto-viscoplastic regimes. For applications of the technique, it is useful to determine the smallest possible representative volume element (RVE). Therefore, a sensitivity study is performed on a 3D High Energy X-Ray Diffraction Microscopy (HEDM) reconstructed Ni-based superalloy where the sub-domains of the full-reconstructed image are used for pointwise comparison of field values between each sub-set and the reference state to evaluate the sensitivity to domain size. The test is repeated on synthetically created 3D microstructures with varying anisotropy factors, showing the sensitivity of the method to both elastic anisotropy and the number of grains per simulation domain. The conclusions of the analysis are used in the application of the method to investigate the mechanical behavior of additively manufactured 2-phase alloys. Statistically representative Ti microstructures are created synthetically, and the FFT technique is used to study the effect of the prior β -grain size, primary α -colony size, the size and shape of the primary α -grains and the volume fraction of α and β on the stress-strain distributions of these 2-phase structures.

Title: Damage Phenomenon in Solid Propellants - Computational Aspects

Author(s): Sebnem Ozupek, Birkan Tunc, *Bogazici U.*

The study aims to predict failure of highly filled elastomers, in particular solid propellants, based on damage accumulated throughout the component service life. Realistic representation of the propellant response based on accurate determination of material model parameters and an efficient numerical algorithm were developed. The constitutive model was implemented in finite element software ABAQUS and was used to perform three dimensional nonlinear viscoelastic simulations. The propellant response was mathematically represented using a nonlinear damaging viscoelastic model. The model is applicable to large deformations and rotations. Softening due to damage and nonlinearities during cyclic loading are accounted for. Both phenomena are formulated through the use of internal state variables. The numerical algorithms for the calibration of the model were illustrated for a solid rocket propellant test data. The procedure requires data from only a small number of relatively easy tests. The formulation and its implementation were validated for a wide range of loading conditions. Simple as well as complex geometries were considered. The results without damage were compared to analysis results using standard ABAQUS material models. The effect of damage was evaluated for all loading conditions. Particular emphasis was given to evaluation of damage model parameters during thermal loading. The predictions for uniaxial and biaxial loadings at constant temperature, and uniaxial loading at transient temperature were compared to the experimental data. The results encourage the employment of the nonlinear viscoelastic stress analysis method to predict the response of the full-scale motor under various operational loadings, in particular cyclic temperature loading which is of particular interest in determining the end of service life.

Title: Structural Arrangements During Plastic Deformations of Amorphous Polymers

Author(s): Alejandro Pacheco, *Uninorte*; Romesh Batra, *Virginia Tech*.

Molecular dynamics simulations have been used to analyze the yielding process during stepped simple tensile/compression loading of bulk amorphous polyethylene at temperatures well below the glass transition temperature. Specimens formed by 20 linear chains of 1000 beads each (20000 coarse grained CH₂ units), with energies described by the united atom potential were deformed at a temperature of 100K. Configurations at axial strains ranging from 0% to 30% were allowed to reach steady state equilibration. Local structural changes were analyzed using two methods: (i) a geometric description by computing the evolution of the self and inter chain entanglements and the free volume, and (ii) the method of Empirical Orthogonal Functions to obtain a reduced description of the displacement field and the nonlinear vibrational modes of the system at each strain level. It was found that at the early stages of deformation the inter-chain entanglement decreased continuously while self-entanglement showed no significant variations. Surprisingly, the energy content of the nonlinear vibrational modes is almost the same for a large portion of the frequency range regardless the imposed strain. These observations are in agreement with the hypothesis of plastic deformations been accommodated at loosely packed regions in the material.

Title: A Gauss-Newton Optimization Method for Material Profile Inversion in 2D Heterogeneous Semi-Infinite Media Using Scalar Waves

Author(s): Alireza Pakravan, Craig M. Newton, *New Mexico State U.*; Jun Won Kang, *Hongik U.*

An inversion framework employing a Gauss-Newton-Krylov optimization method is implemented to reconstruct material profiles in 2D heterogeneous semi-infinite solid media using SH waves. In particular, a full-waveform inversion approach is used to image the shear wave velocities in a layered media using a hybrid finite element formulation developed using scalar waves. Perfectly-Matched-Layers (PMLs) wave absorbing boundaries are introduced to limit the semi-infinite extent of the solid medium. Using the transient wave equations conjunction with the anti-plane constitutive relation and the PML, a partial-differential-equations (PDEs)-constrained optimization method is implemented that leads to a classic KKT (Karush-Kuhn-Tucker) system comprising time-dependent state, adjoint, and time-invariant control problems. The system for the optimal solution of material properties is resolved by a reduced space approach based on a line search algorithm where the search direction is computed by the Gauss-Newton method. Numerical results are presented that show the reconstruction of shear wave velocity profiles of a two-dimensional layered system. The performances of the Gauss-Newton and Fletcher-Reeves methods are compared in terms of their efficiency in reconstructing the material profile.

Title: Ballistic Impact Performance Evaluation of Advanced Combat Helmet Using Numerical Methods

Author(s): Emre Palta, Hongbing Fang, David C. Weggel, *U. North Carolina-Charlotte.*

Combat helmets are crucial safety gears that are needed for personal protection of army soldiers and law enforcement officers. Combat helmets had a long history of usage and development and modern combat helmets have evolved from steel to composite woven fabrics to improve protection and comfort. The U.S. Army adopted the Advanced Combat Helmet (ACH) in the early 2000s as a primary combat helmet. Due to difficulties of conducting experimental studies for ballistic impacts on body armors, numerical modeling and simulations provide an alternative solutions to closely study the ballistic performance of the ACH. However, challenges still exist for modeling ballistic impact problems due to the nature of high-speed contacts, nonlinear large deformations, and fractures in the computational methods. In this study, nonlinear finite element (FE) modeling and simulations were used to study the performance of the ACH under various ballistic impacts. The ACH model was first validated using test data provided by the manufacturer, which were conducted to fulfill requirements of the NIJ-0106.01 standards [1] and V50 ballistic limit evaluation [2]. The comparison of simulation results to experimental data showed that the ACH model developed in this study is capable of predicting the ACH responses under ballistic impacts with reasonably good accuracy. Finally, a case study was performed to evaluate the performance of ACH under impacts of a 9-mm and a higher caliber bullet. A field ballistic experiment was also conducted in this case study to validate the ACH model. A comparison of simulations results with experimental data showed that the ACH model had reasonably good accuracy in predicting the ACH responses in both impact simulations. References [1] NIJ (1981), "Ballistic Standard for Ballistic Helmets", U.S. Department of Justice National Institute of Justice, Standard -0106.01. [2] Department of Defense Test Standards, (1997), "Military Specification: Helmet, Ground Troops and Parachutists." MIL-H-44099A

Title: A DLM/FD/IB Method for Simulating Compound Vesicle Motion Under Creeping Flow Condition

Author(s): Tsorng-Whay Pan, Roland Glowinski, *U. Houston.*

In this article we present first a new distributed Lagrange multiplier/fictitious domain (DLM/FD) method for simulating fluid-particle interaction in Stokes flow. A conjugate gradient method driven by both pressure and distributed Lagrange multiplier, called one-shot method, has been developed to solve the discrete Stokes problem while enforcing the rigid body motion within the region occupied by the particle. The methodology is validated by comparing the numerical results of a neutrally buoyant particle of either a circular or elliptic shape with the associated Jeffery's solutions. We have successively combined the above methodology with an immersed boundary (IB) method and an elastic membrane modeled by a spring network to simulate the dynamics of a compound vesicle. In simple shear flow under creeping flow condition, the results are consistent with those obtained in literature. In Poiseuille flow, the compound vesicle motion is dominated by the motion of the vesicle membrane as expected and stays in the central region of the channel.

Title: A Cut Cell Finite-Element Method for Problems in Linear Elasticity

Author(s): Sushrut Pande, Panayiotis Papadopoulos, *UC Berkeley*.

This talk presents the development of a cut cell based Finite Element Method to solve problems in linear elasticity. In present practice finite element analysis relies heavily on unstructured meshes that fit the boundary of the domain over which the partial differential equation is solved. This approach is both time consuming and dependent, often crucially, on the quality of the mesh. This work attempts to overcome this challenge by instead solving the equation over a Cartesian axis-aligned grid which is not fitted to the boundary of the domain. The domain is first immersed inside a regular grid. Cells of this grid are then classified according to their relative position to the boundary (inside, outside, or partial) and the exterior elements are trimmed away eventually resulting in a bounding box of the domain. Approaches for imposing the Dirichlet and Neumann boundary conditions are developed in two and three dimensions using information from the partial cells. For Dirichlet boundary conditions, the nodes of partial cells lying outside the domain are projected onto boundary points of the domain, where the boundary conditions are strongly enforced pointwise. For Neumann boundary conditions, the boundary of the domain is approximated by a piecewise linear curve, and the boundary conditions are applied in a weak sense using a local least-squares minimization approach. The method is tested on a range of problems from linear elasticity in two and three dimensions whose analytical solutions are known. For Dirichlet and Neumann boundary conditions, it is observed that this method attains the same asymptotic convergence rates as those achieved by unstructured mesh finite element methods.

Title: Active Muscle Response on Occupant-Knee Airbag Interaction in Automotive Impacts

Author(s): Matthew Panzer, Bingbing Nie, Jeff Crandall, *U. Virginia.*

Knee airbags (KABs) have been implemented in many vehicles as a countermeasure that can potentially reduce occupant lower extremity injuries. However, it was previously demonstrated that the risk of lower extremity increase can increase in out-of-position occupants interacting with a deploying KAB, and the ensuing kinematics are highly sensitive to the initial position of the legs relative to the KAB. This study builds on that previous study by investigating how active muscle response of the occupant may influence the loading and kinematics of the legs during a KAB deployment. An LS-Dyna finite element model of the human body (THUMS Version 4.0.1) was modified to include the 32 Hill-type active muscles in the lower extremities. Active muscle response in the human model was implemented to produce three actions: passive (no activation), braking (700N in right leg only), and bracing (700 N in both legs). Simulation cases were conducted in frontal and oblique impact scenarios with KAB deployment, and a full factorial simulation matrix was generated based on the following variables: seat position (standard/seat-forward), muscle response (passive/braking/bracing), vehicle condition (static/frontal impact/oblique impact), and KAB type (rear-deploy/bottom-deploy/no airbag). The corpuscular particle method was used to generate the dynamics of the unfolding and inflating of the KAB. Changes to the biomechanics and injury risk of the occupant model were examined with respect to these factors. Simulation results showed that muscle activation did not have substantial effect on the resulting external kinematics of the lower extremities in each loading scenario. However with muscle activation, the internal forces developed in the lower extremities were almost 100% higher than in passive muscles cases. A seat-forward position also resulted in an increase in the loads of the tibia and femur, and would result in a significant amount of lower extremity abduction and less KAB coverage. The rear-deployed KABs also resulted in higher lower extremity forces than the bottom-deployed type KABs in the seat forward condition. The oblique crash conditions generated higher lower extremity forces on the driver's left leg than in the frontal crash condition, with no significant changes to the response in the driver's right leg. These preliminary results confirm a number of hypotheses on the biomechanics of occupant-KAB interaction that have been raised within the automotive safety community to explain the real-world crash statistics that suggest that KABs may increase the risk of lower extremity injury to occupants rather than decrease the risk as designed.

Title: Polyhedral Meshing in Industrial Applications: Achievements and Challenges

Author(s): Stefano Paoletti, *CD-Adapco*.

This talk will cover practical algorithms for generating polyhedral meshes in 3d suitable for simulations. Polyhedral meshing is that branch of mesh generation that concerns itself with cells or elements formed by an arbitrary number of faces. The faces themselves can be formed by an arbitrary number of vertices. The polyhedral cells are therefore the most general simply connected type of cells that can be used in numerical simulations. The known methods available to build a polyhedral mesh are relatively few and refer to the concept of a Voronoi cell. The Voronoi cells can be generated either directly or indirectly, dualising a primal Delaunay tetrahedral mesh. Although a direct creation of Voronoi cells would seem the simplest way to generate a polyhedral mesh, most of the available software rely on the indirect method: the dualisation. The motivation is twofold: on the one hand much efforts have already been spent in developing fast and robust Delaunay-based tetrahedral meshers, on the other hand the dualisation can be applied, at least in theory, to any mesh. In reality even a Delaunay tetrahedral mesher does not generate meshes that satisfy the Delaunay properties everywhere. In particular at the boundary of the mesh, non-Delaunay cells are generated to honor the input triangulation. Therefore a method that does not strictly require primal Delaunay cells has advantages. However, once the Delaunay property of the primal cells is lost, the dual cells are not Voronoi cells any more. In particular the dual faces are not planar and are not orthogonal to their primal edges, the dual cell itself can be non-convex. This scenario requires remedies in the form of mesh optimization, that can take two different and concurrent paths: pre and post dualisation techniques. Before the dualisation the primal mesh should be topologically optimised removing the low-valence vertices. After the dualisation the dual mesh needs the removal of the non-convex cells and a vertex-movement-based optimisation based on quality metrics specific to the physics solved in the simulation. Significant effort has been spent in developing concave cells “splitters” that cut the non-convex cells in two or more convex pieces. The definition of quality metrics that can be used on a general mesh, and therefore on a dual mesh, is still a field of active research together with the development of effective methods to globally optimise the mesh according to the chosen set of quality metrics.

Title: Bayesian Uncertainty Quantification, Validation and Propagation for Large-Order Models in Structural Dynamics

Author(s): Costas Papadimitriou, Costas Argyris, *U. Thessaly*.

Bayesian inference is used for quantifying and calibrating uncertainty models in structural dynamics based on vibration measurements, as well as propagating these uncertainties in simulations for updating robust predictions of system performance, reliability and safety. The Bayesian tools are based on Laplace methods of asymptotic approximation and sampling algorithms. These tools involve solving optimization problems, generating samples for tracing and then populating the important uncertainty region in the parameter space, as well as evaluating integrals over high-dimensional spaces of the uncertain model and loading parameters. They require a moderate to very large number of system re-analyses to be performed over the space of uncertain parameters. For high-fidelity finite element models required in real-world applications, the use of Bayesian technique may result in excessive computations. The computational challenges for Bayesian uncertainty quantification and propagation of large-order linear and nonlinear models in structural dynamics are addressed. High performance computing techniques are integrated with Bayesian techniques to efficiently handle large-order models of hundreds of thousands or millions degrees of freedom, nonlinear actions activated during system operation, and stochastic loads. Fast and accurate component mode synthesis (CMS) techniques are proposed, consistent with the finite element model parameterization, to achieve drastic reductions in computational effort. Surrogate models are also used within multi-chain MCMC algorithms with annealing properties to substantially speed-up computations [1], avoiding full system re-analyses. Significant computational savings are also achieved for highly-parallelized operation in system simulations and sampling algorithms by adopting the $\Pi 4U$ software [2] to efficiently distribute the computations in available multi-core CPUs. The proposed Bayesian computational framework for reconciling high-fidelity models and experimental data in system simulations is applicable to diverse fields of engineering sciences. The importance of the proposed computational framework is demonstrated for applications on model-based structural damage identification of civil infrastructure. Acknowledgements: This research has been implemented under the "ARISTEIA" Action of the "Operational Programme Education and Lifelong Learning" and was co-funded by the European Social Fund (ESF) and Greek National Resources. References [1] Angelikopoulos, P., Papadimitriou, C. and Koumoutsakos, P. "X-TMCMC: Adaptive kriging for Bayesian Inverse Modeling." *Computer Methods in Applied Mechanics and Engineering*, accepted for Publication. [2] Hadjidoukas, P.E., Angelikopoulos, P., Papadimitriou, C. and Koumoutsakos, P. (2015). " $\Pi 4U$: A High Performance Computing Framework for Bayesian Uncertainty Quantification of Complex Models." *Journal of Computational Physics*, 284(1), 1–21.

Title: Solution of Large-Scale Problems in Structural Analysis: Monte Carlo Simulation vs. Spectral Stochastic Finite Element Method

Author(s): Manolis Papadrakakis, George Stavroulakis, Dimitris G. Giovanis, Vissarion Papadopoulos, *Nat'l. Techn'l. U. Athens.*

The most straightforward techniques of solving stochastic partial differential equations (PDE) are the widely applicable non-intrusive Monte Carlo (MC) methods. They can handle any type of problems (linear, nonlinear, dynamic) as well as any kind of uncertainty in the load or in the system properties. In particular, when dealing with deterministic external loading, MC methods feature the solution of successive linear systems with multiple left-hand sides, since only the coefficient matrix K changes in every simulation. On the other hand, recently proposed approaches, such as stochastic collocation and Galerkin methods, are intrusive and are using tensor product spaces for the spatial and stochastic discretizations. The present work revisits the computational performance of non-intrusive Monte Carlo versus intrusive Galerkin methods for large-scale stochastic systems in the framework of high performance computing environments. The purpose of this work is to perform an assessment of the range of the relative superiority of these approaches with regard to a variety of stochastic parameters. In both approaches, the solution of the resulting algebraic equations is performed with a combination of primal and dual domain decomposition methods implementing specifically tailored preconditioners. The solution of repeated simulations of the Monte Carlo method is accelerated with an A-orthogonalization procedure aiming at reducing the iterations of subsequent simulations, while the solution of the augmented equations of the stochastic Galerkin method is enhanced with preconditioners which combine the block diagonal features of the resulting matrices as well as the sparsity pattern of the off block-diagonal terms.

Title: Dynamic Simulation of Hydraulic Fracturing Using XFEM

Author(s): Matin Parchei Esfahani, Robert Gracie, *U. Waterloo.*

A fully coupled dynamic extended finite element (XFEM) model for the process of hydraulic fracturing is presented in this research. Fluid flow is modeled using the general Reynold's lubrication theory in which Darcy flow is assumed within the fracture network, and into the permeable matrix. The flow is considered to be dynamic, and interacting with the solid matrix only through the internal fracture boundaries. The fluid model is coupled with a fractured solid rock model in which local nonlinear plastic processes around the fracture front (process zone) are taken into account using a cohesive fracture model with the appropriate traction-separation law. The resulting set of nonlinear equations is solved for the solid-fluid interaction parameters that are locations and velocities of the fracture and fluid fronts, as well as distribution of the fracture aperture and fluid pressure along the fracture length. An Eulerian finite element discretization is employed for the hydro-dynamic equations in conjunction with an enriched Lagrangian XFEM discretization for the fractured solid equations, and an explicit (i.e. central difference) scheme for the time integration. The model is finally validated using some laboratory test results on Polymethyl methacrylate (PMMA) specimens.

Title: Simulating Unsteady Flow Over a NACA0021 Airfoil in Deep Stall with PyFR

Author(s): Jin Seok Park, Freddie Witherden, Peter Vincent, *Imperial College London*.

High-order numerical methods for unstructured grids offer the promise of increased simulation accuracy in the vicinity of complex engineering geometries. The Flux Reconstruction (FR) approach [1] provides a unifying framework for various unstructured high-order methods, including discontinuous Galerkin and spectral difference schemes. Moreover, FR methods exhibit a significant degree of temporal/spatial locality, which is favourable when considering recent hardware architectures, such as Graphical Processing Units (GPUs). PyFR (www.pyfr.org) [2] is an open-source Python based framework for solving advection-diffusion type problems using the FR approach. It is able to solve compressible inviscid and viscous flow problems on a range of modern platforms, including heterogeneous mixtures of CPUs and GPUs. In this talk, we will demonstrate how PyFR can be applied to simulate unsteady flow over a NACA0021 airfoil in deep stall, at a Reynolds number of 270,000. Various important metrics will be compared with experimental data, including time-averaged lift/drag coefficients, and temporal force spectra. Particular attention will be paid to the importance of (numerical) aliasing driven instabilities - which can occur when simulating turbulent flows - and the cost/accuracy/robustness pay-off of various anti-aliasing approaches will be discussed. Finally, we will detail the performance/scalability of PyFR for this problem on up to ~100 Nvidia K20 GPUs. [1] Huynh, H. T., A Flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods, AIAA Paper 2007-4079, 2007. [2] Witherden, F. D., Farrington A. M., Vincent P. E., PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach, *Computer Physics Communications*, 185(11) pp. 3028-3040, 2014.

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Title: Atomistic Modeling at Experimental Strain Rates and Time Scales

Author(s): Harold Park, *Boston U.*

I will present a new computational approach that couples a recently developed potential energy surface exploration technique with applied mechanical loading to study the deformation of atomistic systems at strain rates that are much slower, i.e. experimentally-relevant, as compared to classical molecular dynamics simulations, and at time scales on the order of seconds or longer. I will highlight the capabilities of the new approach in uncovering new, mechanical force-induced unfolding pathways for the protein ubiquitin, while also discussing potential differences with experimental data regarding whether ubiquitin unfolds via an intermediate configuration.

Title: Combined Isotropic-Kinematic Hardening Law Based on Two-Yield Surface for Asymmetric/Anisotropic Yielding and Hardening

Author(s): Taejoon Park, Farhang Pourboghrat, *Michigan State U.*; Kwansoo Chung, *Seoul Nat'l. U.*

A combined type isotropic-kinematic hardening law based on two-yield surface plasticity and nonlinear kinematic hardening was developed, which accounts for asymmetry/anisotropy in yielding and hardening. Applying combined type laws for both the inner and (outer) bounding yield surfaces, the Bauschinger and transient behaviors as well as permanent softening and hardening stagnation during reverse loading were accounted for. As for the yield function, J2 based non-quadratic asymmetric/anisotropic function was generalized along with the non-associated flow. Especially for the transient behavior such as cyclic hardening at a low strain range (without back stress reversal) and out-of-phase hardening (the so called latent hardening or cross-loading), the bounding surface was designed to temporarily expand and recover to its original size in this new law. As for the asymmetry/anisotropy in yielding and hardening, full isotropic hardening law based on the evolutionary yield function was also considered and compared with the developed combined isotropic-kinematic hardening law. The developed constitutive law was characterized for advanced high strength steels and applied to the spring-back validation for 2-D draw bending.

Title: An Efficient Algorithm for 3D Multi-Material Topology Optimization Problems

Author(s): Jaejong Park, Alok Sutradhar, *Ohio State U.*

While most of the problems in the topology optimization consider optimization of two material phases i.e. material and void, this work introduces an efficient method that can handle multiple material phase optimization problems in 3D space. An alternating active-phase algorithm where the problem at hand is divided into a series of the traditional material-void topology optimization subproblem is employed for the multi-material problem. A simple block coordinate descent method similar to Gauss-Seidel technique is used to solve the subproblems. The alternating active phase is improved with the multi-resolution scheme. Three distinct levels of discretization are used to represent the displacement, design variable, and density fields. This assures higher resolution designs for the solutions. A projection scheme is utilized to compute element densities from design variables to control the length scale of the members in the solutions. Results of several numerical examples show the efficacy of the proposed implementation. The abovementioned multi-material algorithm can also be applied to design of high performance microstructures with multiple materials. Using inverse homogenization, desired material properties can be achieved in the solutions of many material design problems. Introducing the multi-resolution scheme incorporated with the multi-material concept into the topology optimization brings limited complexity but also opens up new opportunities for designers and engineering regardless of subjects as it provides crisp potential design alternatives that are not often intuitive.

Title: A Waveform Relaxation Newmark (WRN) Method for Structural Dynamics

Author(s): Marco Pasetto, Jiun-Shyan Chen, *UC San Diego*; Haim Waisman, *Columbia U.*

The Newmark family of methods is one of the most popular numerical integration schemes for the solution of the systems of ordinary differential equations arising from linear structural dynamics problems. Its implicit implementation is unconditionally stable but requires the inversion of a coefficient matrix, which makes it computationally expensive; its explicit form, on the contrary, has a low computational cost as it does not have to compute the inverse, but it is conditionally stable, thus limiting the allowed time increment. Furthermore, these methods are structured in the time domain and not well suited for parallel implementations due to unavoidable processor communication at every time step. This work proposes a Waveform Relaxation Newmark (WRN) algorithm for the solution of linear second-order hyperbolic systems of ODEs in time, which retains the unconditional stability of the implicit Newmark scheme with the advantage of the lower computational cost of explicit time integration schemes. This method is also unstructured in the time domain and is very well suited for parallel implementation. Firstly, the basic waveform relaxation method is reviewed and the derived iterative WRN algorithm is presented, along with the solution of one-dimensional model problems to analyze the accuracy of the proposed scheme. We consider a Jacobi and Gauss-Seidel type splitting and study their convergence. Lastly, the performance of the WRN algorithm is compared to a standard implicit implementation of the Newmark's method (trapezoidal rule) and the results obtained confirm the effectiveness of the Waveform Relaxation Newmark algorithm as a new class of more efficient integrators.

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Title: Finite Elements for Accurate, Large-Scale Quantum Mechanical Materials Calculations: From Classical to Enriched to Discontinuous

Author(s): John Pask, LLNL.

We discuss recent developments in finite-element (FE) based methods for the solution of the Kohn-Sham equations that have made possible smaller basis sets and larger calculations than possible by current state-of-the-art planewave (PW) based methods, in some cases by an order of magnitude or more. Such gains are crucial in the context of quantum molecular dynamics simulations, which can require in excess of a year to complete using large-scale parallel computational platforms. We begin with classical FE based approaches, demonstrating optimal convergence rates and micro-Hartree agreement with established PW based methods. We then discuss recent enriched partition-of-unity FE (PUFE) methods, which build known atomic physics into the basis while retaining strict locality and systematic improvability. By incorporating known physics, these bases can achieve the required accuracies with an order of magnitude fewer degrees of freedom (DOF) than required by traditional PW based methods, for "hard atom" calculations in particular. However, with such enrichment comes more expensive quadrature and some degree of ill-conditioning, which we address. By incorporating not only local-atomic but also environmental physics into the basis, recent Discontinuous Galerkin (DG) based approaches can achieve larger reductions in DOFs still, while retaining both strict locality and systematic improvability. Crucially, however, the DG formulation allows for orthonormality as well, alleviating conditioning issues and allowing for the solution of standard rather than generalized discrete eigenproblems in the critical N^3 scaling step of the Kohn-Sham solution. Accurate quantum mechanical forces have also been demonstrated. We conclude with an outlook and particular applications interests going forward.

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Title: Analysis of the Error in an Iterative Algorithm for Solution of the Regulator Equations for Linear Distributed Parameter Control Systems

Author(s): Thanuka Pathiranage, *Texas Tech U.*

The regulator equations are a coupled pair of operator equations that arise in the geometric approach to regulation in systems and control. The primary regulator problems of interest in this work involve asymptotic tracking and disturbance rejection for linear parabolic distributed parameter systems. Underlying our approach to solving problems of this type is the geometric regulation methods in which control laws are obtained by solving a pair of regulator equations. In general it is not easy to solve the regulator equations or even obtain accurate numerical solutions. Furthermore, our main results apply to tracking and disturbance rejection for very general smooth bounded reference and disturbance signals. In this paper we present the β -iteration method for obtaining approximate solutions of the dynamic regulator equations for a class of infinite dimensional linear control systems. A major advantage of this theory compared to previous work is that an explicit error analysis is available for each step in the iteration. In particular, the geometric convergence of the β -iteration error can be controlled by changing β . We demonstrate our estimates on a variety of control problems in multi-physics applications.

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Title: Numerical Error in Model Evaluation and its Effect on Surrogate Construction

Author(s): Abani Patra, Hossein Aghakhani, *U. Buffalo*; Elaine Spiller, *Marquette U.*

This talk will examine the effect of numerical error on the construction of statistical surrogates (e.g. GaSP emulation). We will use dual weighted error estimation as additional source of information in the construction of the surrogate and illustrate the impact of the numerical error on use of the surrogate to quantify uncertainty. We will examine these questions in the context of a challenging hyperbolic transport model of geophysical mass flows.

Title: Equilibrium Maps of Nanostructures

Author(s): Subrahmanyam Pattamatta, Ryan Elliott, Ellad Tadmor, *U. Minnesota.*

Traditional atomistic simulation techniques are unable to address systematically the inherent randomness in nanostructure response to external stimulus and are limited to unrealistically high loading rates. We describe a new method that addresses both issues through the construction of an "Equilibrium Map" (EM). The EM, simply put, is the collection of all possible nanostructure configurations as function of the applied external load. The EM is used to construct dynamically meaningful response trajectories to external stimulus at any rate. A high-performance implementation for EM generation has been developed and applied to study the behavior of a nanoslab of nickel atoms under compression. The results are startling in their complexity and consistent with experimental observations.

Title: A Concurrent Parallel Multi-Scale Algorithm for Large 3D Continuum/Atomistic Simulations with Applications to Dislocations

Author(s): Fabio Pavia, W. A. Curtin, *EPFL*; B. A. Szajewski, *Brown U.*

Deformation and fracture processes in engineering materials often require simultaneous descriptions over a range of length and time scales, with each scale using a different computational technique. Here we present a high-performance parallel 3D computing framework for executing large concurrent multiscale studies that couple an atomic domain, modeled using molecular dynamics, and a continuum domain, modeled using explicit finite elements. The coupling is achieved with the robust Coupled Atomistic/Discrete-Dislocation (CADD) method. The key features here are the extension to 3D and, moreover, an implementation within the parallel molecular dynamics code LAMMPS that enables use of all the tools associated with this popular open-source code. As an example, we show the application of our multiscale method by discussing robust results obtained from an atomic scale analysis of the dislocation line tension with two distinct interatomic potentials and demonstrating an effective Peierls Stress applicable to curved dislocation structures. Our multiscale method allows us to reproduce the results of extremely large atomistic simulations at a much lower computational cost, thus enables us to remove the finite size effects normally influencing small finite-size atomistic simulations.

Title: A High-Performance Computing Approach to the Simulation of the Coupled Fluid-Multibody Dynamics Problems

Author(s): Arman Pazouki, Dan Negrut, *U. Wisconsin-Madison.*

Motivated by the desire to investigate subsea applications, we provide a framework for the simulation of the fluid--solid interaction problems. The simulation approach relies on an explicit--implicit, Lagrangian-Lagrangian (LL), solution to the coupled Navier--Stokes and Newton-Euler equations of motion. The main components of the simulation framework include: (i) A fluid dynamics engine to solve the momentum and continuity equations. Herein, a weakly compressible Smoothed Particle Hydrodynamics (SPH) method is employed for the simulation of the fluid dynamics in a Lagrangian framework. The time integration of the equations of motion, which are represented as Ordinary Differential Equations (ODE), is handled via a second order Runge-Kutta scheme; (ii) A general multibody dynamics framework that supports impact, contact, and constraint. The constrained multibody dynamics framework relies on a Differential Variational Inequality formulation of the contact problems, which are augmented by algebraic constraints to mimic the joints and couplings. In a time stepping approach, the constraints impulses and objects velocities are evaluated using an Accelerated Projected Gradient Descent (APGD) algorithm, and used later to update the generalized coordinates; (iii) An interface model relying on ghost markers is used to resolve the motion of the solid objects in the fluid domain via a two-way fluid--solid coupling. The fluid--solid communication at the interface is updated after any position update, i.e. at every step of the Runge-Kutta scheme, to maintain the order of accuracy. Although being simpler to solve, the ODEs resulted from fluid dynamics dominate the bulk of the computation due to the sheer number of Lagrangian markers required to capture the physics of the fluid. Therefore, a high performance computing approach is leveraged to balance the computational load between the fluid and solid domains.

Title: The Complex Optimum of Trabecular Bone Structure

Author(s): Darin Peetz, Ahmed Elbanna, *U. Illinois, Urbana-Champaign.*

As the fields of biomimetic materials design and topology optimization continue to develop, the appeal of recreating biological structures through optimization techniques grows. Many of these investigations focus on the trabecular structure of bones, which is considered to be a self-optimizing structure in accordance with Wolff's law. However, while the structure's adaptations to changing stress patterns have been well documented, its optimality for compliance is less certain (Sigmund, 2002). Given the complexity of many biological systems, it is expected that these structures serve several purposes. One such purpose widely cited as a secondary motivation to compliance minimization is fluid conductivity. Several studies have combined compliance minimization with a minimum constraint on member surface area which produces a large number of thin "struts" in the optimal design. The increased surface area is essential for self-healing of the structure, as deconstruction/reconstruction of the members originates on the surface (Seeman & Delmas, 2006). These studies largely neglect the reduced stability of these thinner members; however, stability is important considering the high stresses on the reduced member sizes. Lack of consideration of stability in these studies may be attributed to the high computational cost. Through efficient coding of an in-house C++ code and parallelization we have managed to make the stability problem comparable to the compliance minimization problem. If computations are limited to a single eigenvalue, the cost is only 2-3 times more than the compliance problem. Our code continues to perform well even if multiple eigenvalues are considered. Despite the increased computational cost, multiple eigenvalues are required to ensure each eigenvalue remains distinct or measures are taken to make them differentiable. Implementing the compliance and stability objectives, in addition to constraints on perimeter/surface area and volume produces results as expected. The compliance objective ensures the structure remains stiff for a given amount of material, and the perimeter constraint gives the structure increased porosity. The addition of stability considerations leads to more complex structures with many braces. By changing the relative weight of the different objectives, several interesting topologies emerge, enabling us to relate structure to function by pointing to the role of different objectives in the emergence of different structural features. Works Cited Seeman, E., & Delmas, P. (2006). Bone Quality - The Material and Structural Basis of Bone Strength and Fragility. *New England Journal of Medicine*, 2250-2261. Sigmund, O. (2002). On the Optimality of Bone Microstructure. *Synthesis in Bio Solid Mechanics*, 221-234.

Title: Study on Damage Evolution Dynamics for the Spall Fracture of Ductile Metal

Author(s): Xiaoyang Pei, *Inst. Fluid Physics.*

The properties of damage evolution dynamics in the spall fracture of ductile metals are studied by theoretical model and simulation. Based on three damage degree, a model of damage evolution dynamics was established in which the process of damage evolution are divided into four stages: nucleation of voids, elastic-plastic growth of voids, complete plastic growth of voids and coalescence of voids. Based on the present model, the experiments were simulated, and the factors that affect the damage evolution dynamics and the parameters in the model were discussed.

Title: Evolutionary Algorithms Applied to Experimental Analysis and Computational Simulation of Magnetorheological Elastomers

Author(s): Jean-Paul Pelteret, Bastian Walter, Jochen Kaschta, Paul Steinmann, *Friedrich-Alexander U.*

Magnetorheological elastomers are smart, field-responsive composite materials that are of increasing interest in numerous industries, with much work being conducted to characterise them. They exhibit microstructural changes under the influence of a magnetic field, namely due to inter-particle and particle-matrix interactions [1]. If it is applied during curing, the migration of the magnetisable particles causes the formation of chain-like structures leading to anisotropic properties of the cured media. Imaging and rheological experiments are performed to quantify the influence of the microstructure. These results lead to the development of phenomenological constitutive models [2] that may be later used in computational analysis. To achieve this, the experiments and material models must be designed correctly such that they highlight and capture the dominant material properties under a large range of environmental conditions. Following this, suitable constitutive parameters must be determined [3]. In this work we explore the use of evolutionary algorithms (EAs), which are metaheuristic optimisation methods, to assist in this regard. The process of determining constitutive parameters is not only semi-automated, but also repeatable. We primarily demonstrate how EAs can be used to help design and test constitutive models, and detect the influence of material composition, deformation and magnetic field on its coupled response. From this we illustrate the correlation between the outcome of rheological experiments and those predicted by analytical and Finite Element approaches. The financial support of the ERC Advanced Grant MOCOPOLY is gratefully acknowledged. [1] M. Jolly and J. Carlson and B. Munoz. A model of the behaviour of magnetorheological materials. *Smart Materials and Structures* 5:607–614, 1996. [2] P. Saxena, J-P. Pelteret and P. Steinmann. Modelling of iron-filled magneto-active polymers with a dispersed chain-like microstructure. *European Journal of Mechanics A/Solids* 50:132–151, 2015. [3] B. Walter, P. Saxena, J-P. Pelteret, J. Kaschta, D. Schubert and P. Steinmann. On The Preparation, Characterisation, Modelling And Simulation Of Magneto-Sensitive Elastomers. In: *Proceedings of the Second Seminar on the Mechanics of Multifunctional Materials*, Bad Honnef, Germany, 5-9 May 2014.

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Title: Combining Dissipative Particle Dynamics, Finite-Element Method and Boundary Element Method to Study Red Blood Cell Diseases

Author(s): Zhangli Peng, *U. Notre Dame*; Qiang Zhu, *UC San Diego*; Igor Pivkin, *U. Lugano*; Ming Dao, *MIT*; George Karniadakis, *Brown U.*

By combining particle-based and continuum-based methods, we investigate the biomechanics of red blood cells (RBCs) and related diseases, such as malaria, anemia and sickle cell disease, for a better understanding of the pathology and development of diagnostic tools. To overcome the computational challenge due to the multiscale feature of RBC mechanics, we apply different numerical methods for different length scales and different conditions. For instance, we applied dissipative particle dynamics (DPD) to simulate the RBC membrane fluctuations and the interaction between RBCs and endothelial cell slits. We applied boundary element method (BEM) to simulate the surrounding shear flow, finite element method (FEM) to simulate the membrane elasticity, Langevin dynamics (LD) to simulate the conformational change of protein complexes, and Monte-Carlo (MC) method to simulate the domain unfolding of individual proteins. By coupling these methods using multiscale modeling approaches, we made important progresses in both applications and fundamental understanding. For example, we discovered that it is easier for mature sexual malaria parasites to transmit than immature ones due to both the unique shape and reduced deformability of their host RBCs. This finding provides a possibility of identifying novel drug targets for malaria eradication. Another example is: we found that the donut-like resting shape of RBCs is due to a unique stress-free initial configuration of the cytoskeleton, which will guide future experiments to measure this stress-free configuration.

Title: Multi-Scale Modeling of the Nanoindentation of Bcc Iron Using QCDFT Method

Author(s): Qing Peng, Suvranu De, *RPI*.

We report our recent study on the mechanical properties of bcc iron through the simulations of the nanoindentation on iron surface using Quasi-Continuum Density Functional Theory (QCDFT) modeling. The QCDFT is a concurrent multiscale method based on the framework of quasicontinuum (QC) approach with DFT as its sole energetics formulation. The local QC energy is calculated by DFT with Cauchy–Born hypothesis and the nonlocal QC energy is determined by a self-consistent embedding approach, which couples nonlocal QC atoms to the vertices of the finite elements at the local QC region. The QCDFT method is applied to a study of nanoindentation on bcc iron with the presence and absence of Carbon impurities.

Title: Sparse Polynomial Chaos Approximation with Gradient-Enhanced L1-Minimization

Author(s): Ji Peng, Alireza Doostan, *U. Colorado*; Jerrad Hampton, .

Gradient-enhanced uncertainty quantification (UQ) has received recent attention, in which the gradients of quantity of interest (QoI) with respect to uncertain parameters computed from, for instance, adjoint equations are used to enhance quality of approximation. Polynomial chaos expansions (PCE) are now standard methods in UQ. When the QoI can be represented by a sparse PCE, L1-minimization, originally proposed in the context of compressive sampling, can identify the PCE coefficients with a number of samples typically smaller than other methods. In this work, we investigate a gradient-enhanced L1-minimization approach, in which the gradient information computed from adjoint equations is applied to enhance the identification of the PCE coefficients. Due to the addition of gradient information to the standard L1-minimization, the existing stability and convergence analysis are, however, inadequate. We analyze the stability and convergence of the gradient-enhanced L1-minimization approach, and provide bounds for the stability and convergence rate for such approximation via Hermite PCE. We demonstrate our analysis empirically via three numerical examples: a manufactured PCE, an elliptical partial differential equation with stochastic coefficients, and a wavy-channel plane-Poiseuille flow.

Title: Three-Dimensional Characterization and Modeling of Microstructure Effects on Nucleation and Growth of Spall Damage in FCC Materials

Author(s): Kapil Krishnan, Sudrishti Gautam, Andrew Brown, Saul Opie, Leda Wayne, Pedro Peralta, Arizona State U..

Shock loading is a complex phenomenon that can lead to failure mechanisms such as strain localization, void nucleation and growth, and eventually spall fracture. Studying spall damage on a microstructural level helps understanding intrinsic material characteristics that lead to damage localization sites and to formulate continuum models that account for the variability of the damage process due to microstructural heterogeneity. Experimental observations in pure polycrystalline Cu indicate that damage tends to localize at grain boundaries (GB) and triple junctions [1]. However, work still has to be done to determine the physics driving the damage at these “intrinsically weak” microstructural sites. The work presented here focuses on the application of a computational model to study the nucleation and evolution of spall damage at the microstructural level [2]. Crystal plasticity [3] along with the Mie-Grüneisen Equation of State (EOS) are implemented and coupled with different damage criteria via a multiplicative decomposition of the total deformation gradient into plastic, damage and elastic components to study the effects of stress concentration and strain localization GBs and triple junctions (TJs). The constitutive model is calibrated using experimental data from single crystal impact experiments, in copper specimens with both planar and perturbed surfaces. The experiments with the latter type of specimens allowed to sample directly the effect of initial yield strength and hardening rate on the evolution of hydrodynamic instabilities, particularly the Richtmyer-Meshkov [4], which is shown to be affected significantly by material anisotropy and led to additional data to select and calibrate a hardening model. The resulting model is then used to model multicrystal impact experiments. The results indicate that strain localization is the predominant driving force for damage evolution at GBs. The results also indicate the voids tend to nucleate predominantly at TJs and other junctions with high grain connectivity. These voids grow along adjacent GBs with tendencies for strain localization. The influence of microstructure on local void nucleation and growth rates is also studied. The simulations show good correlation with the experimental results. 1. Peralta, P., DiGiacomo, S., Hashemian, S., et al: *Int. J. Damage Mech.*, 2009. 18: p. 393-413. 2. Krishnan, K., Brown, A., Wayne, L., et al.: *Met. Mat. Trans. A*, 2015: p. 1-12. 3. Luscher, D.J., Bronkhorst, C.A., Alleman, C.N., and Addessio, F.L.: *J. Mech. Phys. Sol.*, 2013. 61(9): p. 1877-1894. 4. Piriz, A.R., López Cela, J.J. and Tahir, N.A.: *Nuc. Instr. Meth. Phys. Research A*, 2009. 606(1-2): p. 139-141.

Title: Evolutionary Design of Natural Laminar Airfoil Coupled to Shock Control Bumps for Drag Reduction Using Pareto, Nash and Stackelberg Games

Author(s): Zhili Tang, Yongbin Chen, *Nanjing U.*; Jacques Periaux, *CIMNE*.

In order to improve the flight performances and to increase cruise time of transonic high aspect ratio aircraft, it is important to investigate computational methods for friction drag reduction. At high Reynolds numbers, Laminar Flow Control technologies and Natural Laminar Flow profile/wing design are both efficient methods which can reduce the turbulence skin friction. However, the existence of wide range of favorable pressure gradient at a laminar flow airfoil surface leads to strong shock waves occurring at the neighborhood of the airfoil's trailing edge. Consequently, the reduction of the friction drag due to the extension of the laminarity surface of the airfoil is competitively compensated with an increase of shock wave induced drag. In this paper, we introduce the transition prediction method based on the "Linear Stability Theory" to predict the transition location of the airfoil. Then a Multi-objective Genetic Algorithm (GAs) coupled with a different games (cooperative Pareto, competitive Nash and hierarchical Stackelberg) is implemented to optimize the airfoil shape with larger laminar flow range and a weaker shock wave drag simultaneously due to a Shock Control Bump (SCB). The associated coupled software can easily capture the Pareto Front, the Nash Equilibrium or the Stackelberg solutions of this Multi-objective optimization problem. The different solutions are analyzed and show aerodynamic performances of airfoils trade offs between the delay of the profile's transition location and the increased intensity of shock wave due the position and shape of a bump installed on the extrados of the airfoil. Results of numerical experiments compare efficiency of the coupled Game-GAs software and design quality of the different solutions. From the analysis/synthesis of results it is concluded that a series of laminar flow airfoils which higher aerodynamic performances can be significantly improved with optimal SBC shape and position when compared to the baseline airfoil. Key words: natural-laminar-flow airfoil, linear stability theory, transition prediction, shock wave reduction, Bump geometries, multi-objective optimization, Genetic algorithms, Pareto Front, Nash Equilibrium, Stackelberg solution

Title: Immersed Boundary Method Based on Hierarchical B-Splines for Fluid-Structure Interaction

Author(s): Chennakesava Kadapa, Wulf Dettmer, Djordje Peric, *Swansea U.*

Fluid-Structure Interaction (FSI) is a complex phenomenon and developing robust numerical schemes for FSI has proved to be a challenging task. The most widely used approach to simulate FSI is to use body fitted meshes enhanced by Arbitrary Lagrangian-Eulerian (ALE) formulation. However, the distortions of the fluid mesh due to the deformations of solid domain limit the applicability of the standard ALE formulations to problems with moderate deformations, and often require sophisticated re-meshing and remapping algorithms for large deformation problems. In this scenario immersed-boundary methods (IBMs) offer a viable alternative. In IBM fluid is typically solved on a regular Cartesian grid on which the solid is free to move and, as fluid mesh is independent of the movement of the solid, there is no need for special mesh moving schemes. In the present work we propose IBM based on hierarchical B-Spline Cartesian grid. One of the main motivating factors behind use of hierarchical B-Splines for the background fluid grid is their local refinement capability. In the area of interest the solution space can be readily enriched by the use of hierarchical B-Splines thereby eliminating the need for expensive global refinement. The immersed solid is represented by a set of Lagrangian points. The standard Galerkin formulation is used to discretise the governing equations and the unconditionally stable and second-order accurate generalised-alpha method is used for time-integration. Performance of the proposed formulation is demonstrated by studying several benchmark problems and by comparing the parameters of interest with the reference values. The methodology is then used to study the performance characteristics of an industrial check-valve and proved to be effective in capturing topology changes during opening and closing stages. Without the need for mesh moving scheme and with the capability to perform efficient local refinement the proposed formulation has proved to be efficient and robust for simulating a range of fluid-structure interaction problems.

Title: Method and Energy Laws for the Unique Identification of Material Properties: Application to the Passive Myocardium

Author(s): Luigi E. Perotti, Aditya Ponnaluri, William S. Klug, Daniel B. Ennis, *UC Los Angeles*; Shankarjee Krishnamoorthi, *Indian Inst. Tech. Gandhinagar*; Daniel Balzani, *TU Dresden*.

Significant changes in the material properties of biological tissue are often associated with disease progression. For example, cancerous tumors or fibrotic tissue depositions have a different stiffness than their healthy tissue counterparts. Modeling the tissue material behavior and identifying its material properties are part of a cogent and emerging diagnostic strategy. As such, it is crucial that the material properties describing differences in tissue stiffness between healthy and diseased states are identified uniquely. However, many currently available methods in the literature do not guarantee a unique identification of the material properties, which limits robustness and contributes to a strong dependence on the initial guess and fine-tuning of the solution algorithm. We propose a new method to model the tissue mechanical response and to identify uniquely its material properties. Fundamental to our approach is the assumption that the full displacement field in the tissue and the applied load causing the deformation are known. The displacement field can be acquired using, for example, magnetic resonance imaging or echocardiography while the applied load may be acquired using different techniques (e.g., heart catheterization to measure intraventricular pressures for cardiac applications). Both measures are routinely acquired for clinical patients. In this setting, there are two key components in our approach: 1) an innovative formulation of the minimization problem to identify uniquely the material properties, and 2) the formulation of the material energy law. In contrast with previous approaches, we define an objective function to minimize the difference between applied and internal forces, rather than between experimental and computed displacements. We also provide a procedure for identifying a material energy law, to be coupled with our solution method, that is able to accurately describe the material behavior in finite kinematics and is polyconvex. Lastly, we present the verification and validation of our method using several examples in the context of passive cardiac mechanics. Changes (i.e., stiffening) in the response of passive myocardium are linked to diastolic heart failure (DHF), a debilitating heart condition affecting more than 50% of heart failure patients in the US. We compare our method and material energy laws with others presented in the literature both at the material point level and in a ventricular geometry. A robust and reliable characterization of a patient's passive myocardium response may help in diagnosing DHF, monitoring its regression, and enabling targeted pharmacological and/or surgical therapies.

Title: HiPOD: Two POD Strategies for a Hierarchical Model Reduction

Author(s): Massimiliano Lupo Pasini, Alessandro Veneziani, *Emory U.*; Simona Perotto, *Politecnico di Milano*.

Reduction of computational costs when solving complex systems of partial differential equations is becoming a crucial issue as scientific computing is extensively used in practical applications. This is particularly true when solving optimization, identification or, in general, inverse problems, when the same set of equations with different values of the parameters or boundary/initial conditions needs to be solved many times. Different methods for reducing the complexity and the size of the numerical problems to be solved have been investigated in the last 15 years. In some cases, the size of the finite dimensional problems obtained after the discretization is reduced by taking advantage of an off-line phase when the solutions for particular configuration of the parameters are computed to provide a basis set in the on-line stage. In other cases, the model to be solved is simplified to obtain an efficient still reliable solver, by properly taking advantage of the features of the problem relevant for the application of interest. In this talk we present a method of model reduction stemming from the combination of these two approaches. We actually combine the Hierarchical Model (HiMod) reduction technique with the well known Proper Orthogonal Decomposition (POD). We call the resulting approach HiPOD. HiMod is a model reduction technique to tackle phenomena with a dominant dynamics, possibly featuring local relevant transverse components, like for blood flow in arteries, air in internal combustion engines, water in rivers, oil in pipes. The idea is essentially to discretize the full model by combining a standard 1D finite element approximation along the main stream with a modal expansion for the transverse directions [1]. POD is a well known approach to reduce the dimensionality of a problem, by identifying its principal components in a set of snapshots computed in the off-line stage. We propose two different approaches, the first one based on a standard POD projection; the second one adopts a two-level POD procedure based on interpolation. In the first case the problem is parametrized by problem coefficients and boundary data, in the latter one we focus on the problem coefficients. The two proposed Hi-POD procedures merge the reliability of a Hi-Mod approximation with the computational efficiency characterizing POD. Even though the HI-POD technique deserves to be investigated in more details from a theoretical view point, the current results are very promising. [1] S. Perotto and A. Veneziani. J. Sci. Comput., 60 (2014), no. 3, 505-536

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Title: Engineered Foams with Tunable Acoustic Properties

Author(s): Fabien Chevillotte, *Matelys* ; Camille Perrot, *U. Paris-Est*, Emmanuel Guillon, *Lafarge Rsch. Centre*.

In a previous paper [J. Acoust. Soc. Am. 134, 4681-4690 (2013)], the authors have described a method for identifying a local geometry model of real double porosity foams related to relatively sharply peaked bubble size distributions which is used to predict their acoustical macro-behavior from X-ray computed microtomography and numerical homogenization techniques. Assuming scale separation between the incident audible sound wave and the largest characteristic size of the pores, the model consists in a three-dimensional periodic unit cell made from a regular arrangement of spherical pores allowed to interpenetrate during the foaming process with a micro-porous matrix. This lecture will propose a parametric study of the microstructure morphology for the pore size, the throat size (i.e. the smallest interconnection between two pores), and the bubble porosity, and will indicate their effects in terms of transport properties and sound absorption at normal incidence. From these structure/property relations, guidelines follow providing optimal design of microstructures compatible with a pre-existing manufacturing process. [Invited lecture]

Title: High-Order Discontinuous Galerkin Simulations on Domains with Large Deformations

Author(s): Per-Olof Persson, Luming Wang, *UC Berkeley*.

We present new high-order accurate methods for moving domains with large deformations [1-2]. The popular Arbitrary Lagrangian-Eulerian (ALE) method can be viewed as a mapping-based approach which, together with appropriate treatment of the Geometric Conservation Law (GCL), allows for arbitrarily high orders of accuracy in both space and time. However, the method requires smooth mappings between the initial (or reference) frame and the actual physical configuration. These can be generated for domains undergoing moderate deformations, such as pitching and heaving airfoils, or structures with small deformations. But many other applications require topological changes to maintain a well-shaped mesh/transformation, e.g. rotating machinery or configurations involving multiple moving objects. In this work, we generate unstructured moving meshes by a sequence of entirely local operations [3]. This produces high-quality meshes throughout the simulation, and provides a simple description of the mesh changes between each timestep. Using this information we can construct efficient numerical schemes based on high-order discontinuous Galerkin formulations, and we consider both space-time and ALE/projection-based methods in 2D and 3D. We demonstrate our framework on a range of problems, including standard verification problems which show that the scheme remains high-order accurate even with complex mesh reconfigurations and frequent edge connectivity changes. We also show a number of flow problems in both 2D and 3D which show the ability of our method to deal with complex domain motions. [1] L. Wang and P.-O. Persson, A High-Order Discontinuous Galerkin Method with Unstructured Space-Time Meshes for Two-Dimensional Compressible Flows on Domains with Large Deformations, in review. [2] L. Wang and P.-O. Persson, High-order Discontinuous Galerkin Simulations on Moving Domains using ALE Formulations and Local Remeshing and Projections, Proceedings of AIAA SciTech (2015). [3] P.-O. Persson, G. Strang, A Simple Mesh Generator in MATLAB. SIAM Review, Vol. 46 (2), pp. 329-345, June 2004.

Title: Eliminating the Pollution Effect in Helmholtz Problems by Local Subscale Correction

Author(s): Daniel Peterseim, *Bonn U.*

We introduce a new Petrov-Galerkin multiscale method for the numerical approximation of the Helmholtz equation with large wave number k in bounded domains. The discrete trial and test spaces are generated from standard mesh-based finite elements by local subscale corrections in the spirit of numerical homogenization. The precomputation of the corrections involves the solution of coercive cell problems on localized subdomains of size mH ; H being the mesh size and m being the oversampling parameter. If the mesh size and the oversampling parameter are such that Hk and $\log(k)/m$ fall below some generic constants, the method is stable and its error is proportional to H ; pollution effects are eliminated in this regime. For reference, see <http://arxiv.org/pdf/1411.7512>.

Title: Quantifying the Effects of Noise on Spinodal-Decomposition: Massively Parallel Framework and a Variational Multi-Scale Treatment

Author(s): Spencer Pfeifer, Baskar Ganapathysubramanian, *Iowa State U.*; Victor Calo, *KAUST*.

We present an investigation into the dynamics of phase separation through numerical simulations of the Cahn-Hilliard-Cook (CHC) equation. This model is an extension of the well-known Cahn-Hilliard equation, perturbed by an additive white noise. While it is far more common to exclude such stochastic inclusions, many studies have shown that certain degrees of random fluctuations are critical for proper resolution of physical phenomena. This is especially true for phase critical systems — particularly throughout the earliest stages of evolution. We perform a comprehensive parametric sweep to evaluate the effects of noise on various early stages of phase-separation and coarsening. To perform this in a computationally efficient manner, we explore a variational multiscale formulation of the CHC equation, utilize higher-order time steppers and integrate this with a massively parallel framework. We show scalability up to 100,000 processors on the BlueWaters machine. Our numerical results suggest that the added noise plays a significant role throughout the early stages of the evolution, while late stage morphologies are only weakly influenced. We observe the noise term to accelerate progress towards phase separation — provided that the stochastic term is discretized and implemented correctly. Further analysis reveals a spectrum of distinct microstructural asymmetries associated with noise amplitude throughout the early stages of evolution. In particular, relatively high magnitudes consistently produce uniformly distributed domains, while low magnitudes yield inconsistent clusters of advanced evolution. This finding has clear implications for tailoring processing conditions involving spinodal decomposition.

Title: Enhanced Turbulent Mixing in the Upper Pacific Equatorial Ocean

Author(s): Hieu Pham, Sutanu Sarkar, Kraig Winters, *UC San Diego*.

After three decades since deep-cycle turbulence was first observed in the Pacific equatorial ocean, the mechanism leading to the enhanced mixing remains mysterious. The turbulence plays an important role in ocean heat budget, and therefore, affects global climate cycle like El Nino and La Nina events. Large-scale ocean models are unable to represent it accurately since the physics of the turbulence is still poorly understood. Observations show that the turbulence occurs preferentially during night time and is theorized to be caused by either breaking internal waves or local shear instabilities. In the present study, a Large-eddy simulation (LES) model is used to investigate the dynamical processes leading to the deep-cycle turbulence. The model includes a background flow similar to the observed ocean, a steady westward wind stress, and a diurnal surface buoyancy flux. An LES of a 3-night period shows the diurnal variability in shear, stratification and turbulence in both the surface mixed layer and the sheared region below. Narrowband isopycnal oscillations and nightly bursts of deep-cycle turbulence are seen to occur at depths well below the surface mixed layer, the two phenomena that have been repeatedly observed in the oceans. The model suggests that the turbulence while occurs at depth is initiated by the relaxing of the surface heating flux in the late afternoon, allowing a region with enhanced shear and low gradient Richardson to form below the surface mixed layer. The enhanced shear descends into the deeper water and causes shear instabilities which result in bursts of deep-cycle turbulence. The dissipation rate during the turbulence bursts is elevated by up to three orders of magnitude. Each bursts is preceded by westward propagating oscillations having a frequency near the local buoyancy frequency and a wavelength in a range of 314-960 m. The model shows that evolution of the deep-cycle turbulence includes Kelvin-Helmholtz-like billows as well as downward penetration of vortices.

Title: Crystal Plasticity-Based Constitutive Modeling for Forming and Service Duties of Metallic Materials

Author(s): Minh-Son Pham, *Carnegie Mellon U.; Nat'l. Inst. Standards & Tech.*; Anthony Rollett, *Carnegie Mellon U.*; Stuart Holdsworth, *Swiss Fed'l. Labs.* ; Adam Creuziger, Mark Iadicola, Youngung Jeong, Jonathan Guyer, Timothy Foecke, *Nat'l. Inst. Standards & Tech.*.

Metallic materials experience complex loading conditions over wide ranges of temperatures and rates during forming and in service. Under such loading conditions, the material responses are associated with the behavior of microstructures over various length scales. This study will demonstrate how in-depth understanding of the behavior of important microstructural features (such as dislocations, point defects and crystallographic texture) can help developing constitutive models to accurately describe the mechanical behaviors of metallic materials during forming and service duties. In detail, we will present the development of constitutive models for multi-step forming and cyclic loading of polycrystals based on the thermally-activated interactions and evolution of dislocations, point defects and texture. In this approach, the thermal dependences are taken into account through the relationships between internal stresses and short-range dislocation interactions. The interactions between dislocations on different slip systems are treated in detail to represent the latent and kinematic hardening. In addition to the introduction of various types of dislocation densities, an evolutionary similitude relationship is proposed in order to reflect the evolution of dislocation substructures. The constitutive model will be then extended to include the interaction between dislocations and point defects in order to model the strain aging and recovery. Furthermore, texture is also incorporated in the constitutive model to better describe the anisotropic behavior. Finally, the capabilities of developed models will be benchmarked against (1) the long-term cyclic responses during variable/constant strain amplitudes cycle fatigue of a steel AISI 316L, and (2) the strain path dependence during multi-step forming of an aluminum alloy AA5754 [1, 2]. Moreover, we will demonstrate that the incorporation of higher-order interactions of dislocations in constitutive relationships can improve the predictions of texture and stress evolutions during multi-axial loading [3].

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Title: Transient Analysis of Airway Lung Tissue Under Mechanical Ventilation

Author(s): Israr Mohammad, Parya Aghasafari, Ramana Pidaparti, *UGA*.

Mechanical ventilation can cause injury to airway lung tissue resulting from air pressure. The complex dynamics of lung tissue environment are still being investigated and although significant research has been done there are still unanswered questions with regards to the transmission of mechanical forces into lung tissues resulting from mechanical ventilation. Even though there have been many studies investigating the effects of long term ventilation with respect to lungs, the connection between the global deformation of the whole lung and the strains reaching the lung tissue has not been studied. This study investigates a three-dimensional model of lung tissue having three layers, created from generations 3-4 in order to estimate the strain/stress levels under mechanical ventilation conditions. Several finite element simulations were carried out using transient analysis. The three layers of lung tissue interact with each other during inflation and deflation of lung was developed. The three layers were modeled using two different set material models; one consists of linear material model for all three layers, the other consists of 2 non-linear material models (Neo-Hookean) and a linear material model. The inner part of lung wall was subjected to transient pressure obtained from airflow simulation from mechanical ventilation breathing. Results show that linear material model will lead to higher maximum stress and strain. Maximum stress and strain from using linear material model is 1.14 and 1.43 times higher than using non-linear material model, subsequently. Although the difference is not significant, the location and the order of stress distribution from higher to lower are quite different. Linear material model results show that maximum stress is located on the inner wall of lung tissue, while non-linear material model had maximum stress on middle layer of lung tissue. The results of this study indicate that a linear material model can lead to different stress/strain environment in relation to the location of maximum stress in comparison to non-linear material model. Currently, coupled fluid-solid interaction studies are being carried out to investigate the stress/strain environment in lungs under mechanical ventilation conditions.

Title: FSI-Modeling of Wind Turbine Blades Including Laminar–Turbulent Transition

Author(s): Thomas Graetsch, Dorothee Pieper, *Hamburg U.* ; Michael Breuer, *Helmut-Schmidt U. Hamburg.*

Fluid-structure interaction (FSI) analysis of wind turbines has become an important field of research in recent years. Most contemporary FSI-analyses consider the wind turbine at rated speed and corresponding angle of attack of the blades. For example, in [1] a 3D FSI analysis of the 3-blade NREL 5-MW turbine at full scale is performed and global data such as the aerodynamic torque of the turbine and blade displacements including tower effects are presented. In the present approach we focus on FSI-modeling of the NREL 5-MW wind turbine blades while considering a larger spectrum of angles of attack of the turbine blades in order to account for different wind loading situations. In contrast to [1] we are also interested in the analysis of local lift and drag coefficients of the turbine blade and the dynamic stall behavior. Here, the modeling of laminar-turbulent transition becomes relevant which is hence taken into account. Since the analysis of lift and drag coefficients requires a fully resolved boundary layer, a very fine grid is applied near the walls avoiding the application of wall functions. That allows detailed investigations on the flow field near the rotor blade including laminar–turbulent transition. In the numerical studies we consider the 3-blade NREL 5-MW wind turbine where the blades consist of DU and NACA profiles. For verification and validation purpose we start with several numerical studies regarding the influence of 2D and 3D profiles modeling the blade, the comparison between FSI and pure CFD-analysis, and the influence of dynamic meshing. Results of 2D analysis including laminar-turbulent transition are compared with experimental data [2]. In the 2D analysis, we also study the influence of the tower, where the profile of the rotor blade and the tower is considered at specific height levels of the turbine. Using the optimal parameter setting obtained in the 2D and 3D profile analysis, we proceed with a 3D CFD- and FSI-modeling of a 120°-symmetry model of the rotor at full scale. Based on our analyses, lift and drag coefficients for different pitch angles of the rotor blade are provided and we find that laminar–turbulent transition modeling is relevant for these simulations. References [1] Hsu MC, Bazilevs Y, Fluid-structure interaction modeling of wind turbines: simulating the full machine, *Computational Mechanics* 50: 821-833, 2012 [2] Timmer WA, van Rooij R, Summary of the Delft University wind turbine dedicated airfoils, *J. Sol. Energy Eng.* 125(4): 488-496, 2003

Title: Custom Finite-Element Simulations Using GPGPU Technology: Towards Faster Patient-Specific Predictions

Author(s): Vukasin Strbac, Nele Famaey, Jos Vander Sloten, *KU Leuven*; David M. Pierce, *U. Connecticut*.

We present an implementation of a nonlinear explicit, displacement-based finite element code and its parallelization using GPGPU technology, applied using modern anisotropic, nearly incompressible constitutive models relevant to soft biological tissues. As clinical practice and even surgical theaters start to embrace simulation technology, the need arises for faster preoperative or intraoperative patient-specific analyses. Using modern computational hardware and techniques we detail an implementation capable of decreasing solution times by a factor of 5-20 or more. The proposed algorithm adopts a total Lagrangian worldview, and uses an explicit, constant-step central-difference integration scheme, cf. [1]. To solve representative boundary value problems and exercise our algorithm, we implement trilinear hexahedra, using either full, selective reduced, or under- integration, the later with perturbation hourglass control [2]. Therein, we implement state-of-the-art anisotropic fiber-reinforced hyperelastic constitutive models, calibrated with experimentally determined parameters, to describe the behavior of human arteries. To ensure efficient parallelization we tailor our algorithm for the newer generation GPGPU technology. For example, force storage routines for the models implemented make use of atomic operations. Furthermore, templated GPU kernels allow for easier switching between single and double precision computations, enabling use of much lower time-steps as sometimes required by the near-incompressibility of the materials or by limits in floating-point representation. We also implement texture memory usage as a template parameter for convenient switching, since the newer generations of GPUs generally prefer utilizing caching subsystems for throughput [3]. Additionally, all global-memory variables with non-random locality are re-organized and padded for faster coalesced accesses. Exemplary simulations show promising results when compared directly to well-established finite element codes. With equivalent results, we reduce solution times by a factor of 5-20 or more depending on the element type and mesh size, indicating significant potential for more efficient and economical analyses. To improve the robustness of our algorithm we are currently implementing mixed u-p- κ element formulations, enabling further optimization in terms enforcing (near) incompressibility without significant reductions in time-step size or stability. We demonstrate that our combination of modern GPGPU hardware and computational methods may soon enable finite element analyses relevant to modern clinical workflows. [1] Joldes et al., *Comput Methods Appl Mech Engrg*, 199:3305-3314, 2010. [2] Tarjuelo-Gutierrez et al., *Med Biol Eng Comput*, 52:159-168, 2014. [3] Nvidia Corp., *CUDA C Best Practices Guide*, 6.5:1-85, 2014.

Title: Assessment of a Method for Predicting Impact- and Impulse-Induced Fires

Author(s): Flint Pierce, *Sandia Nat'l. Lab.*

Many impact events involving transportation vehicles are followed by a fire, which frequently represents a significant thermal event. The transportation fuel is typically the main source of combustible in these events. The fuel is often dispersed rapidly in the initial impact, with the primary physics governing the dispersion being inertial forces and the interaction of the fluid with the structure. At later times, the governing physics transitions as gravitational, surface tension, viscous shear, and drag forces become increasingly important. We have defined a method to predict the results of this class of problems that involves initializing a fluid mechanics simulation with the results from a finite element structural dynamics code. The structural code uses a smoothed particle hydrodynamics (SPH) representation for the fluid mass. The SPH results are parsed and evaluated based on dimensionless length-scale and energy criteria to create a time-dependent input condition for the Lagrangian-Eulerian dilute-spray computational fluid dynamics (CFD) reacting flow code. Enabling models in the CFD code include a break-up model and a liquid surface impact model. Limited data exist to validate the methodology. The capability has been demonstrated for five scenarios in past work, and these are used as context to assess the sensitivity of the predicted results to various model input parameters. This presentation will introduce the modeling methods, describe the accuracy of the method when compared to the limited available data, and assess model sensitivity to the drop impact and shatter model that has recently been included in the CFD code.

Title: Computational Mechanics Applied to the Simulation of Fabrics

Author(s): Paulo M. Pimenta, Alfredo Gay Neto, *U. São Paulo*; Peter Wriggers, *Leibniz U. Hannover*.

In this work, we developed a methodology to simulate fabrics using beam elements. The fabric is supposed to be composed by the weft and the warp. Both are modeled using beam elements to represent threads. The beam elements utilized may handle large deformation and finite rotations, using a geometrically-exact formulation. Initially, all the threads, which compose the fabric, are constructed in a given plane. In a first load-step, the warp threads are prescribed to displace such that they assume a wave shape, which will characterize the fabric. This action eliminates the interferences between the threads, initially present. In a second load-step, the prescribed displacement is released. This causes the warp to get in contact with the weft. Then, we used a contact model between beams using a surface-to-surface approach to enforce this constraint. At the end of this second load-step one has already the fabric structure, with all interactions between threads naturally considered. Then, simulations of other loading actions such as tension, compression, bending, torsion, etc. can be performed in order to quantify equivalent properties of the fabric. In a future work, these properties will be used to compound an orthotropic shell model. By now, the model is still in a premature phase, but already shows promising results. The cross section of all threads is considered to super-elliptical. This can be used to create different cross section shapes, from circular, elliptical or even almost-rectangular cross sections. The algorithms were implemented in the GIRAFFE finite element code, under development at the University of São Paulo.

Title: An Energy-Based Approach for Finite Element Modeling of Collagen-Swelling Interaction

Author(s): Peter Pinsky, Xi Cheng, Steven Petsche, *Stanford U.*

The corneal stroma, the principal structural layer of the cornea, like other soft, highly-hydrated and charged collagenous tissues such as cartilage and intervertebral disc, is a polyelectrolyte gel consisting of a mixture of interacting fluid, solid and ionic phases. We take the cornea as a representative connective tissue and propose a new structural modeling approach for the in vivo cornea by explicitly treating it as an electrolyte gel, accounting for the three-dimensional organization of collagen fibers and for collagen-swelling interaction. Current finite element-based models for hydrated connective tissues treat the volumetric behavior of the tissue by assuming incompressible or nearly-incompressible elasticity. This approach is convenient but cannot describe the swelling behavior of the tissue or its steady-state volumetric compressibility. On the other hand, modeling by use of triphasic theories introduces numerical challenges that render the approach too impractical for realistically complex problems. The aim of the current work is to explore a novel energy-based approach for characterizing the tissue osmotic pressure and bulk behavior and to assess its suitability as a basis for efficient finite element approximation. Conditions of thermodynamic equilibrium are assumed to hold, rendering fluid and ionic fluxes time-independent. Such an approach has utility when the long-time, steady-state response to surgical alteration or disease processes is desired. The stromal electrolyte gel free energy is additively decomposed into components which characterize the behavior of the tissue under general deformations. For the ex vivo cornea, we use the mean-field approximation of the Helmholtz free energy for a binary electrolyte which measures the energy of fixed charge, the osmotic energy of mobile ions in a Boltzmann distribution, and the dielectric free energy. To account for active endothelial ionic transport in the in vivo cornea, we show that the stromal mobile ions satisfy a modified Boltzmann distribution, and leading to a modified free energy. Under reasonable assumptions we obtain an analytical form for the modified free energy functional which is convex in volume dilation and provides the key variational ingredient for the finite element formulation. The approach can be easily implemented within a standard finite element framework using only the displacement field. The collagen-swelling model is employed to predict free and confined swelling of stroma in an ionic bath. Swelling resulting from surgical alteration is predicted for the first time. Corneal swelling in Fuch's corneal dystrophy is employed as an illustration of how the model can be adapted to certain pathological conditions.

Title: Influence of the Fracture Process on the Mechanical Behaviour of the Metal Matrix Composites

Author(s): José Pituba, Ágatha Florêncio, Gabriela Fernandes, *Fedr'l. U. Goiás*; Eduardo Souza Neto, *Swansea U.*

This work presents a study about the influence of the fracture process on the mechanical behaviour of the Metal Matrix Composites [1] using a two-dimensional meso-scale model [2]. The matrix zone is modelled by Von Mises elasto-plastic model with linear strain hardening. The elastic inclusions are added to the material in order to improve the mechanical properties of the material. In rupture stages, some microcracks are created mainly in the interface zone surrounding the inclusions. Therefore, it is adopted a modified cohesive fracture model in order to simulate the cracking process until complete failure. The interface zone, surrounding the inclusions, is modelled by means of cohesive contact finite elements in order to capture the effects of phase debonding and interface crack closure/opening. All simulations in this work have been performed by employing the computational homogenization under the plane stress assumption in small strain regime [2]. The average stress is obtained by imposing the macro-strain over the Representative Volume Element and subsequently solving the microscopic initial boundary value problem for the defined boundary condition assumed. The analyses are performed under two different boundary conditions: linear and periodic boundary displacement fluctuations. In summary, the proposed homogenization-based model is found to be a suitable tool for the identification of macroscopic constitutive response of this kind of material. [1] Azizi, R. Micromechanical modeling of damage in periodic composites using strain gradient plasticity. *Engineering Fracture Mechanics*, vol. 92, pp. 101-113, 2012. [2] Fernandes, G. R., Pituba J. J. C., de Souza Neto, E. A. Multi-scale modelling for bending analysis of heterogeneous plates by coupling BEM and FEM. *Engineering Analysis with Boundary Elements*, v. 51, p. 1-13, 2015.

Title: Capturing Multi-Scale Thermo-Structural Effects with a Parallel Generalized Finite-Element Method

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

The computational modeling of intense, localized, nonlinear thermo-mechanical effects in structures poses a challenge in many engineering applications. Localized thermo-mechanical gradients can be introduced by, for instance, concentrated external heat sources or internal material interfaces. High local solution fidelity is required to capture strong temperature and stress/strain gradients; however, localized, fine-scale effects may have a profound impact on the global structural response. Thus, methods used in numerical simulations must address the intrinsic coupling of scales. While hp-adaptive methods are optimal for this class of problems, for realistic, three-dimensional structural models, mesh adaptivity may be prohibitively expensive. To treat the class of problems of interest, this work extends the Generalized Finite Element Method (GFEM) for analysis of three-dimensional, coupled physics problems exhibiting localized heating and thermo-mechanical effects. The method is based on the GFEM with global-local enrichment functions (GFEMgl) [1, 2], which involves the solution of interdependent global and local problems to resolve localized behavior at the structural scale. Because of the high fidelity necessary to resolve localized solution behavior in the neighborhood of sharp temperature and stress/strain gradients, local or fine-scale problems may prove expensive to solve monolithically. Thus, an extension of the GFEMgl which enables the resolution of fine-scale effects by solving many smaller, computationally manageable local problems in parallel is also discussed. Several examples demonstrating the capabilities of the method in resolving localized, nonlinear, three-dimensional thermo-mechanical effects are presented. The accuracy and computational cost of the method in parallel are studied in detail, and strategies for improving the accuracy and efficiency of the method in bridging fine-scale features to the structural scale are also investigated. REFERENCES [1] P. O'Hara, C.A. Duarte, T. Eason, Generalized finite element analysis of three-dimensional heat transfer problems exhibiting sharp thermal gradients, 198(21-26), (2009), 1857–1871. [2] C.A. Duarte, D.-J. Kim, Analysis and applications of a generalized finite element method with global-local enrichment functions, 197(6-8), (2008), 487–504.

Title: Singularity-Free Dislocation Dynamics in Anisotropic Gradient Elasticity

Author(s): Giacomo Po, *UCLA*.

The singular nature of the elastic fields produced by dislocations presents conceptual challenges and computational difficulties in the implementation of discrete dislocation-based models of plasticity. In this work we consider theoretical and numerical aspects of the non-singular theory of discrete dislocation loops in a particular version of Mindlin's anisotropic gradient elasticity with up to six independent gradient parameters. The framework models anisotropic materials where there are two sources of anisotropy, namely the bulk material anisotropy and a weak non-local anisotropy relevant at the nano-scale. The Green tensor of this framework, which we derive as part of the work, is non-singular and it rapidly converges to its classical counterpart a few characteristic lengths away from the origin. Therefore, the new Green tensor can be used as a physical regularization of the classical Green tensor. The Green tensor is the basis for deriving a non-singular eigenstrain theory of defects in anisotropic materials, where the non-singular theory of dislocations is obtained as a special case. The fundamental equations of curved dislocation loops in three dimensions are given as non-singular line integrals suitable for numerical implementation using fast one-dimensional quadrature. These include expressions for the interaction energy between two dislocation loops and the line integral form of the generalized solid angle associated with dislocations having a spread core. The six characteristic length scale parameters of the framework are obtained by independent ab-initio calculations. Several applications of the theory are presented.

Title: A Consistent Homogenization Theory and Numerical Implementation for a Higher Order Plasticity Model from Meso to Macro

Author(s): Leong Hien Poh, Van Tung Phan, *Nat'l. U. Singapore.*

Classical plasticity models, being scale independent, cannot capture any size dependent behavior. One remedy is to adopt a gradient plasticity model at the sub-granular (meso) scale to account for the different micro-processes leading to the various size effects. In this contribution, we adopt, at the meso scale, the isotropic gradient plasticity model by Gurtin (2004) which incorporates the plastic rotation effect, hence enabling it to mimic the behavior of an analogous crystal plasticity model with multiple slip systems (Poh and Peerlings submitted). However, discretization has to be done at a sub-granular level in order to capture the direct influence of grain boundaries. For a typical problem, the computational cost may become prohibitive. This motivates a novel homogenization theory that translates the isotropic plasticity model from meso to macro (Poh 2013). We first impose the Hill-Mandel condition to extract the homogenized governing equations. Departing from most homogenization approaches, we furthermore impose the equivalence of energy and dissipation across the two scales in order to determine the macroscopic constitutive relations. The scale translation is thus thermodynamically consistent, with the three length scale parameters – the intrinsic length scale, the grain size and the characteristic structural length scale – manifesting themselves in the homogenized solutions. This allows for a direct study on the interaction and competition between the different micro-processes, with a significantly lower computational cost compared to a detailed crystal plasticity model. It is also highlighted that the homogenized model recovers a micromorphic continuum, though the difference in our approach is emphasized: the homogenization theory is a bottom-up approach which does not require any constitutive assumptions at the macro level a priori. The numerical framework of the homogenized plasticity model is presented, and the close match between the homogenized solutions and those obtained from detailed meso analyses demonstrated. References: Gurtin, M.E., 2004. A gradient theory of small-deformation isotropic plasticity that accounts for the Burgers vector and for dissipation due to plastic spin. *J. Mech. Phys. Solids* 52, 2545-2568. Poh, L.H., 2013. Scale transition of a higher order plasticity model – A consistent homogenization theory from meso to macro. *J. Mech. Phys. Solids* 61, 2692-2710. Poh, L.H., Peerlings, R.H.J., Submitted for publication. On the role of plastic rotation in an isotropic gradient plasticity model at the meso scale.

Title: Understanding Prismatic Dislocation Loops in Mg by Means of Large-Scale Ab-Initio Simulations

Author(s): Mauricio Ponga, Kaushik Bhattacharya, Michael Ortiz, *Caltech*.

Density Functional Theory (DFT) have been played a significant role in accurately predicting many aspects of materials behavior over the last two decades. DFT reduces the many-body Schrodinger equation of interacting electrons into an equivalent problem of non-interacting electrons in an effective mean field that is governed by electron-density greatly reducing the complexity of the original problem. A major drawback, however, is that the complexity of DFT equations scale to the cube with the number of electrons in the system making the calculation of large samples prohibitively expensive. To tackle this challenge, a number of linear scaling have been developed exploring different properties of the density matrix, spectral quadratures, etc. However, in the study of crystalline defects, an extra challenge is encountered since the concentration of defects is as low as part per million atoms or less and linear scaling does not suffice this issue. In this work, we present a coarse-graining approach for the DFT without *ad hoc* assumptions, spurious physics or significant loss of accuracy. The CG-DFT method is based on a linear scaling method and a spatial reduction of the computational domain through judicious kinematic constrains. The spatial discretization is taken to be dense near defects, but coarse in the vast regions of asymptotic decay. This adaptive mesh discretization greatly reduces the size of the problem with little loss of accuracy leading to a sublinear scaling. The CG-DFT approach is implemented in our computational platform, MacroDFT, and validated with different test problems involving defects in Mg-HCP. After validating the method and implementation we study the nucleation and stability of prismatic dislocation loops in Mg. We will perform a thorough study of the mechanisms that create such loops and will present how they can be used to reduce the basal dislocation mobility in Mg.

Title: A Variational Framework for Electromechanical Viscoactive Constitutive Modeling of the Heart

Author(s): Aditya Ponnaluri, Luigi Perotti, William Klug, *UC Los Angeles*.

A rigorously validated electromechanical heart model would be useful for identifying physiological mechanisms and effective diagnostic and treatment strategies for heart disease. In this study, drawing from the work of Ortiz and Stainier [1] in viscoplasticity, we present a novel constitutive modeling framework for contractile cardiac mechanics, by formulating a single variational principle from which incremental stress-strain relations, and kinetic rate equations for active contraction and relaxation can all be derived. The variational framework straightforwardly accommodates the hyperelastic behaviors measured experimentally for relaxed and contracted tissue, along with the rate- and length- dependent generation of contractile force. We prescribe a three-element, Hill-like model that unifies the “active tension” and “active deformation” approaches. As in the latter approach, we multiplicatively decompose the total deformation gradient into active and elastic parts, with the active deformation parameterizing the contractile Hill element. We adopt as internal variables the fiber, cross-fiber, and sheet normal stretch ratios. The kinetics of these internal variables are modeled via definition of a kinetic potential function derived from experimental force-velocity relations. To model the myocytes activation, the kinetic equations are coupled with the calcium transient obtained from a cell electrophysiology model. At a material point level, we demonstrate the stress-strain curves representative of a single muscle fiber. Further, using these constitutive equations with the finite element method and an ellipsoidal heart geometry, we model the four stages of the cardiac cycle. We evaluate different passive and active strain energy laws, viscous coefficients, force-velocity relationships, and electrophysiology conditions to identify characteristic changes in the gross contraction of the heart. We validate the model via measures such as EF, twist, apex-to-base shortening, fiber shortening, and wall stresses. [1] Ortiz, Michael, and Laurent Stainier. "The variational formulation of viscoplastic constitutive updates." *Computer methods in applied mechanics and engineering* 171.3(1999):419-444.

Title: Characterization and Identification of a Cohesive Zone Model for the Adhesion of Plasma Sprayed Coating on Brittle Substrate

Author(s): Elodie Pons, Guillaume Huchet, Jean-Louis LONGUET, *CEA, DAM, Le Ripault* ; Rafaël Estevez, *SIMaP, U. Grenoble*.

Interfacial cracking is a recurrent failure mechanism observed in multilayer structures and coating systems, in various fields as microelectronics, biomedical engineering, aerospace or new technologies for energy. Delamination between two materials is usually due to their different nature, mechanical and thermal properties and their dissimilar thicknesses. According to the aimed application and operating loadings, a minimum adhesion of the interface is necessary. The CEA Le Ripault studies the mechanical strength and the adhesion properties of various plasma sprayed coatings, whose plasma sprayed ceramic and metallic coatings respectively on ceramic and composite substrates. One of the main difficulties for the characterization of adhesion is the small thickness of each layer (top coating is about 300-700 micrometers, and the substrate is about millimeters). Otherwise, in the "plasma sprayed metallic coating / composite substrate" system, a thin polymer underlayer (about 50-150 micrometers) is inserted to improve coating adhesion. Another feature of these assemblies is the brittleness and the low deformability (less than 1%) of its components. All these constraints limit the choice of standard methods for adhesion tests. Firstly, the materials constituting the stack are characterized separately to identify their mechanical response. In order to fully characterize the adhesion, it is necessary to scan different loading mode through various adhesion tests by applying different loadings and related mode mixity on the interface. Therefore, in addition to traditional tensile strength measurements (mode I), new adhesion criterion have been identified: a shear strength with a configuration test that promotes mode II, an interfacial adhesion energy under mixed mode by means of a notched four-point bending tests and an interfacial adhesion energy close to mode I by wedge tests. The geometry of the specimens was adjusted and optimized according to the adhesion tests implemented. Alongside these experimental measurements, a modeling of all these tests is performed by using the finite element code ABAQUS in order to predict the cracks initiation and propagation along the interface under consideration. To this end, a cohesive model is used to describe the delamination, and more especially a linear traction-separation law is adopted for interface debonding. A methodology to identify the cohesive parameters is presented, based on the experimental data. This approach allows to model failure scenario in good agreement with experimental observation. Thus, the integrity of the assembled structure can be assessed.

Title: Feeding the Beast: Pragmatic Environmental Data Retrieval for Today's Simulation Models

Author(s): Dharhas Pothina, *USACE ERDC*.

As the size and complexity of today's environmental simulation models increases, so does their appetite for data. Environmental data is required both for setup of initial conditions, driving the model through boundary conditions and for verification and validation. The good news is that in today's cloud centric world, there are many high quality hydrological and climatological datasets available on the web. This availability does not however translate into ease of use. In fact, each dataset is usually structured uniquely with distinct mechanisms for querying and for data delivery. Usually, over time, a research lab or modeling community develops a set of scripts to download a particular subset of data that is required for the projects they are currently working on. This works well once the scripts are in place but the system can be fragile. The scripts are usually tied to one architecture or model and data for a particular geographic location and it can be cumbersome to add new datasets or to share the scripts with collaborators. In many model applications, it is common for a major portion of the work to lie in simply assembling the data. Obtaining new datasets is often tedious and error-prone. Many attempts have been made to improve this situation, often through the specification of standards and use of new technologies such as web services. They mostly fail, by either getting bogged down in the complexity of finding a common representation capable of encompassing all possible datasets or by requiring the world at large to change delivery techniques to conform to their approach. Neither approach is scalable. In this talk, we present how we are building a more sustainable approach to data retrieval at ERDC to build the Environmental Simulator project: Ulmo, an open source python library for clean, simple and fast access to public hydrology and climatology data. Ulmo was originally developed as the backend of <http://waterdatafortexas.org> and is now being used as the backend of the Data Services Library at ERDC. Ulmo currently supports several data services including CUAHSI WaterOneFlow services, USGS National Water Information System web services, datasets from the National Climatic Data Center as well as raster services such as the National Elevation Dataset and the National Land Cover Dataset.

Title: The Benefit of Geometrical Personalization on Pedestrian FE Model Response in Vehicle-Pedestrian Impact

Author(s): David Poulard, Huipeng Chen, Matthew Panzer, *U. Virginia.*

Pedestrian finite element models (PFEM) are used to investigate and predict the injury outcomes from vehicle-pedestrian impact. Due to the sensitivity of injury and response of the pedestrian to the relative relationship between pedestrian anthropometry and vehicle geometry, it is believed that PFEM with a generic anthropometry (e.g., 50th percentile male) cannot be sufficiently evaluated against post-mortem human surrogate (PMHS) test data from a wide range of sizes and shapes. Model personalization via geometric morphing can reduce the geometric error of the computational model. The goal of the current study was to evaluate the benefit of personalized PFEM on the biomechanics of vehicle-pedestrian impact. The AM50 THUMS pedestrian model was morphed to the anthropometric specifications of each of four diversely-shaped PMHS used in a series of vehicle-pedestrian impact tests (height range: 1540-1820 mm; weight range: 46-114 kg). The morphing procedure was based on a Dual Kriging interpolation process using control points constructed from external anthropometric measurements. The baseline THUMS model and the four morphed THUMS models were integrated with a mid-sized sedan FE model validated for pedestrian impact up to 40 km/h. A quantitative assessment of the response of the PFEM compared to the experiments was performed on bone kinematics, forces, accelerations, strain gauges and torso deformation. PFEM responses showed good correlation with the PMHS response for the reaction forces, the rib strain, and the overall kinematics. Morphing was found to greatly alter the reaction forces, deflections and the strain time histories in terms of magnitude and phase. The trend observed in the responses of the morphed THUMS indicates that the relative distance between the pelvis and the bumper played a substantial role in the subjects' response. The four morphed models sustained between 3 to 5 rib fractures for the same test, confirming the initial hypothesis that the morphing influenced the injury outcome predicted by the simulation. This study suggests that the response of PFEM in frontal sled tests is sensitive to the geometry, and that a large variation in the number of predicted injuries can be linked to the differences in the subject anthropometry. Although this conclusion does not necessarily apply to PMHS tests, it indicates that the geometry should be carefully quantified during the experiments and the evaluation of PFEM should take into account the variation in the geometry.

Title: Fast Solvers for Sparse Matrices Using Low-Rank Approximations

Author(s): Hadi Pouransari, AmirHossein Aminfar, Eric Darve, *Stanford U.*

Modern simulation codes are attempting to solve increasingly difficult problems, either because of their size and complexity of the geometry, or because of their multi-physics nature, which often leads to coupled PDEs of different types. As a result, many traditional iterative methods no longer work well, and often exhibit slow convergence. In this talk, we will present a new class of preconditioners based on low-rank approximation and hierarchical matrices. The matrices arising from spatial discretization of some partial differential equation in a physical domain are large, but very sparse. Iterative solvers are widely used in many scientific codes to deal with such large sparse linear systems. However, iterative solvers suffer from highly problem dependent pre-conditioner requirement to achieve a reasonable convergence performance. Our preconditioners are based on approximate LU factorizations of the sparse matrices. These methods are applicable to a large family of sparse matrices arising from scientific calculations. The complexity is close to linear with the number of non-zeros in the matrix. As in hierarchical matrices, e.g., the fast multipole method, we decompose the unknowns hierarchically. We then proceed through the usual LU factorization. As we are progressing, fill-in occurs in the matrix. This fill-in is then compressed using low-rank factorizations. The sparsity pattern of the matrix is preserved by introducing new unknowns (the "multipole" and "local" coefficients) [1,2]. A key property of this process is that after eliminating all the leaf unknowns, we are left with a new sparse matrix, of smaller size (the hierarchical tree has one less level), but which has a sparsity pattern similar to the original one. As a result, we can repeat this process, until all levels in the hierarchy have been eliminated. We will present applications relevant to computational fluid dynamics, in which solving the discretized Poisson equation for pressure is the most computationally intensive part of an incompressible Navier-Stokes solver. In particular, we will focus on cases where the density of the fluid varies by orders of magnitude, leading to ill-conditioned linear systems. References: [1] Ambikasaran, Sivaram, and Eric Darve. "The Inverse Fast Multipole Method." arXiv preprint arXiv:1407.1572 (2014). [2] Aminfar, Amirhossein, Sivaram Ambikasaran, and Eric Darve. "A fast block low-rank dense solver with applications to finite-element matrices." arXiv preprint arXiv:1403.5337 (2014).

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Title: A Constitutive Model for Martensitic Phase Transformation Plasticity in Advanced High Strength Steels

Author(s): Taejoon Park, Farhang Pourboghrat, *Michigan State U.*; Kwansoo Chung, *Seoul Nat'l. U.*

A constitutive law was developed based on the rate-independent crystal plasticity to account for the mechanical behavior of advanced high strength steels. The texture evolution of ferrite, martensite and retained austenite was represented by slip deformations on their active slip systems. As for the retained austenite, martensitic phase transformation induced by the plastic deformation was also considered based on the lattice invariant shear deformation and the orientation relationship between parent austenite and transformed martensite. Considering the effect of stress state and temperature, the optimized plastic deformation of the retained austenite among the various available deformations for the martensitic phase transformation was decided to have the minimum-energy associated with the work during the phase transformation. The developed constitutive law was numerically formulated and implemented into the commercial FE code with the aid of user-defined material subroutine and ultimately applied to the representative volume element (RVE) simulations.

Title: An Integrated Seismic-Motion Forward Solver for the Study of Topographic Amplification Effects in Large Sedimentary Basins

Author(s): Babak Poursartip, Loukas F. Kallivokas, *UT Austin*.

Seismic hazard assessment relies increasingly on ground motion numerical simulations, since recent advances in numerical methods and computer architectures make it ever more practical to obtain the surface or near-surface response to real/idealized or realistic seismic events. The key motivation stems from the need to access the performance of sensitive components of the civil infrastructure (nuclear power plants, bridges, lifelines, etc), when subjected to realistic scenarios of seismic events. We discuss an integrated approach that deploys best-practice tools for simulating seismic events in arbitrarily heterogeneous formations, while also accounting for topography. Specifically, we describe an explicit forward wave solver based on a hybrid formulation that couples a single-field formulation for the computational domain with an unsplit mixed-field formulation for Perfectly-Matched-Layers (PMLs and/or M-PMLs) used to limit the computational domain. Due to the material heterogeneity and the contrasting discretization needs it imposes, an adaptive time solver is adopted. We use a Runge-Kutta-Fehlberg time-marching scheme that adjusts optimally the time step such that the local truncation error rests below a predefined tolerance. We use spectral elements for spatial discretization, and the Domain Reduction Method to allow for the efficient prescription of the input seismic motion. We discuss the components of the integrated approach we followed, and report the results of parametric studies for various idealized topographic features, which show motion amplification and de-amplification that depends, as expected, on the relation between the topographic feature's characteristics and the dominant motion wavelength. Since discrepancies between recorded and simulated seismic surface motion have been observed and often attributed to topographic effects, it is also of interest to be able to assess the motion involving real surface topographies: we report results involving three-dimensional simulations in complex physical terrains.

Title: Peridynamic Modeling of Carbon Nanotube Reinforced Polymer Nanocomposites

Author(s): Naveen Prakash, Gary Seidel, *Virginia Tech.*

Composite materials reinforced with carbon nanotubes are being increasingly researched for their unique mechanical, thermal and electrical properties. Carbon nanotubes which are known for high strength and stiffness properties, enhance macroscale structural properties even at low volume fractions. To fully understand how these fillers reinforce the matrix material, a thorough understanding of CNT – polymer interactions at the nanoscale is required. In this work, we used peridynamics to study computationally CNT reinforced composite materials at the nanoscale. Traditionally the finite element method has been used as a computational tool, but when dealing with discontinuities such as fracture, FE methods often have issues of resolving the crack surface and mesh sensitivity. Peridynamics, a non – local continuum theory is being increasingly used as a method to treat problems with fracture, especially in dynamic loading conditions. The non – local nature of the theory ensures that the same equations can be applied on and off discontinuities such as cracks. The mechanical properties of CNT reinforced composite materials in the transverse direction (perpendicular to alignment of CNTs) are highly dependent on the polymer properties and CNT – polymer interface properties. We consider a unit representative volume element at the nanoscale with hexagonal packing of CNTs in a polymer matrix phase. The interface is characterized by interface bonds connecting polymer and carbon nanotube particles and the stiffness is considered to be some function of the properties of the two phases. The response of the RVE under quasi - static and dynamic loading conditions is studied for different types of interfaces. In addition, for a better representation of the interface, traction separation data from molecular dynamics simulations of a polymer – CNT interface is used to characterize the interface bonds and effect of this characterization is presented.

Title: Cost Reduction via Domain Simplification in the Karhunen-Loève Expansion

Author(s): Srikara Pranesh, Debraj Ghosh, *Indian Inst. Sci.*

In probabilistic mechanics the heterogeneity in material properties is often modeled using random fields. For computational purpose these random processes or fields need to be discretized. The Karhunen-Loève (KL) decomposition is one widely used discretization method, where the eigenfunctions of the covariance kernel are used as the bases. Finding these eigen-functions requires solving a Fredholm integral equation of second kind. Traditionally this integral equation is solved using a finite element (FE) method, where often the mechanics mesh is reused. This step is not only computationally expensive, but is also associated with the question whether an optimal FE mesh for the mechanics problem is also optimal for discretizing the random field. Another interesting question is whether the geometric shape of the physical domain should have any effect on the KL discretized random field. Based on these questions, in this work it is first mathematically proved that the KL expansion is domain independent. That is, irrespective of the shape or size of the spatial domain, the realizations of the field from the KL expansion remain invariant — although the individual KL coefficients may vary. Based on this observation, a new method of computation of the KL coefficients is proposed here. Accordingly, first the original spatial domain is replaced by a minimal bounding box. Then the integral equation is solved over this new simplified domain using standard quadrature. Through numerical studies in two and three dimensions it is demonstrated that the proposed method is significantly faster than the traditional FE method, the speed gain can go up to four orders of magnitude. A mathematical estimate on the truncation error is also presented.

Title: Adaptive Resolution Simulation of Polarizable Supramolecular Water Models

Author(s): Julija Zavadlav, Matej Praprotnik, *Nat'l. Inst. Chem., Slovenia*; Manuel Nuno Melo, Siewert J. Marrink, *U. Groningen-Netherlands*.

Multiscale particle-based simulation methods, such as Adaptive Resolution Scheme (AdResS) [1], are becoming increasingly popular due to their significant computational advantage with respect to conventional atomistic simulations. For these kind of simulations it is essential to develop accurate multiscale water models that can be used to solvate biophysical systems of interest. Recently, a multiscale simulation of water with 4-to-1 mapping was performed where four semi-harmonically connected SPC (Simple Point Charge) waters were mapped to a MARTINI water site [2]. Simulation of a protein embedded in such solvent was shown to give no notable differences compared to the fully atomistic simulation [3]. Here, we extend the supramolecular mapping to coarse-grained models with explicit charges. In particular, the two tested models are the polarizable water (PW) and big multiple water (BMW). We show that our approach leads to the correct reproduction of the relevant structural and dynamical properties. The developed multiscale solvents are compatible with the popular MARTINI force field and can therefore be readily used to solvate various biomolecular systems. [1] M. Praprotnik, L. Delle Site and K. Kremer, *Annu. Rev. Phys. Chem.* 59, 545 (2008). [2] J. Zavadlav, M. N. Melo, A. V. Cunha, A. H. de Vries, S. J. Marrink and M. Praprotnik, *J. Chem. Theory Comput.* 10, 2591–2598 (2014). [3] J. Zavadlav, M. N. Melo, S. J. Marrink and M. Praprotnik, *J. Chem. Phys.* 140, 054114 (2014).

Title: A Novel Iterative Solver for Large, Sparse Linear Systems

Author(s): Phanisri Pratapa, Phanish Suryanarayana, *Georgia Inst. Tech.*; John Pask, *LLNL*.

We develop a novel approach for accelerating the classical Jacobi iterative method for the solution of large, sparse linear systems. We verify the accuracy and efficacy of the proposed approach in a range of test cases, including nonsymmetric systems of equations. We demonstrate that the proposed technique possesses a favorable scaling with system size that is accompanied by a small prefactor, even in the absence of a preconditioner. In particular, we show that the developed technique is able to accelerate the classical Jacobi iteration by over four orders of magnitude, with speed-ups that increase as the system gets larger. Moreover, we find that it significantly outperforms the Generalized Minimal Residual (GMRES) method in the range of problems considered here, with the relative performance again improving with size of the system. Overall, the proposed method represents a simple yet efficient technique that is particularly attractive for large-scale parallel solutions of linear systems of equations.

Title: Application of a Constrained Mass-Conservative Generalized Multiscale Finite Element Method to Flow Models

Author(s): Michael Presho, *UT Austin*.

In this presentation, we propose a method for the construction of locally conservative flux fields through a variation of the Generalized Multiscale Finite Element Method (GMsFEM). The flux values are obtained through the use of a Ritz formulation in which we augment the resulting linear system of the continuous Galerkin (CG) formulation in the higher-order GMsFEM approximation space. In particular, we impose the finite volume-based restrictions through incorporating a scalar Lagrange multiplier for each mass conservation constraint. This approach can be equivalently viewed as a constraint minimization problem where we minimize the energy functional of the equation restricted to the subspace of functions that satisfy the desired conservation properties. To test the performance of the method we consider equations with heterogeneous permeability coefficients that have high-variation and discontinuities, and couple the resulting fluxes to a two-phase flow model. The increase in accuracy associated with the computation of the GMsFEM pressure solutions is inherited by the flux fields and saturation solutions, and is closely correlated to the size of the reduced-order systems. In particular, the addition of more basis functions to the enriched multiscale space produces solutions that more accurately capture the behavior of the fine scale model. A number of numerical examples are offered to validate the performance of the method.

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Title: Faults Simulations for Three-Dimensional Reservoir-Geomechanical Models with the Extended Finite Element Method

Author(s): N. Sukumar, *UC Davis*; Jean Prevost, *Princeton U.*

Faults are geological entities with thicknesses several orders of magnitude smaller than the grid blocks used to discretize reservoir and/or over-underburden geological formations. Introducing faults in a complex Reservoir and/or Geomechanical mesh therefore poses significant meshing difficulties. In this work, we introduce faults in the mesh without meshing them explicitly, by using the extended finite element method (X-FEM) in which the nodes whose support intersects the fault are enriched. For the Geomechanics, the fault is treated as an internal displacement discontinuity that allows slipping to occur using a Mohr-Coulomb type criterion. For the Reservoir, the fault is an internal fluid flow conduit that allows fluid flow in the fault as well as to enter/leave the fault. In the X-FEM, the framework of partition of unity is used to enrich the nodes. The faults are represented by enriching the displacement approximation with a discontinuous (Heaviside) function, whereas the approximation for the fluid pressure includes functions that admit a discontinuity in their normal derivative across the fault. The procedure has been implemented in 2D and 3D, for both structured and unstructured meshes. Examples that demonstrate the versatility and accuracy of the procedures will be presented. Also, the influence of the rate of loading on activation of faults will be demonstrated.

Title: A Recovery-Based A-Posteriori Error Estimator for Linear Fracture Mechanics in the framework of the Stable Generalized Finite Element Method (SGFEM)

Author(s): Rafael Lins, Manoel Denis Ferreira, Sergio Proenca, *U. Sao Paulo*; Carlos Armando Duarte, *U. Illinois, Urbana-Champaign*.

In this study the recovery-based [1] a-posteriori error estimator proposed in [2] is investigated in the framework of the Stable Generalized Finite Element Method (SGFEM) [3]. The SGFEM is chosen mainly due to the robust solution provided by the method to the ill-conditioning of the G/XFEM. The Heaviside functions and special functions taken from fracture mechanics are adopted as enrichment functions in the SGFEM. Therefore, the recovered stresses can incorporate the discontinuities and the singularities introduced by the crack. Some necessary adjustments to adapt the expression defining the enhanced stresses in the original error estimator, [2], to the SGFEM framework are discussed. For instance, in the hereby proposed approach both the Heaviside and the linear Heaviside enrichment functions are incorporated in the recovered stresses, therefore modifying the related expression in the original estimator. Relevant aspects such as effectivity indexes, error distribution, convergence rates and accuracy of the recovered stresses are used in order to demonstrate the effectiveness of the error estimator. We selected two benchmark problems of the 2-D fracture mechanics to assess the robustness of the error estimator hereby investigated. All the numerical results are presented for both G/XFEM and SGFEM. The main findings of this investigation are: the SGFEM shows higher accuracy than G/XFEM and relative reduced sensitivity to blending element issues. Moreover, the error estimator can accurately capture these features of both methods. REFERENCES: [1] O.C. Zienkiewicz and J.Z. Zhu. A simple error estimator and adaptive procedure for practical engineering analysis. *International Journal for Numerical Methods in Engineering*, 24:337-357, 1987. [2] C. Prange, S. Loehnert and P. Wriggers. Error estimation for crack simulations using the XFEM. *International Journal for Numerical Methods in Engineering*, 91:1459-1474, 2012. [3] V. Gupta, C.A. Duarte, I. Babuška and U. Banerjee. A stable and optimally convergent generalized FEM (SGFEM) for linear elastic fracture mechanics. *Computer Methods in Applied Mechanics and Engineering*, 266:23-39, 2013.

Title: Adaptive Surrogate Modeling for Bayesian Parameter Estimation of RANS Models

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

Bayesian inference for parameter estimation can rapidly become prohibitive in the case of complex models. We consider here an adaptive model reduction approach based on a pseudo-spectral method to lower computational cost. We therefore propose to extend our latest work on error decomposition and adaptive refinement for response surfaces [1,2] to the development of surrogate models that can be substituted for the full models to estimate the parameters of Reynolds-averaged Navier-Stokes models. The error estimates and adaptive schemes are driven here by a quantity of interest and hence rely on the approximation of an adjoint problem. We also show that the method can be used to estimate evidences for model selection. The methodology is illustrated on the Spalart-Allmaras RANS model for turbulence simulation [3]. [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] C.M. Bryant, S. Prudhomme, and T. Wildey, "A posteriori error control for partial differential equations with random data", *SIAM Journal on Uncertainty Quantification*, Submitted (2013). Available as ICES Report 13-08 (2013). [3] P.R. Spalart and S.R. Allmaras, "A one-equation turbulence model for aerodynamic flows", *Recherche Aéronautique*, Vol. 1, pp. 5-21 (1994).

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Title: Automating the Characterization of Materials Thermodynamics and Kinetics Using Ab Initio-Based Cluster Expansion Hamiltonian Methods with CASM

Author(s): Brian Puchala, John Thomas, *U. Michigan*; Anton Van der Ven, *UC Santa Barbara*.

Cluster expansion effective Hamiltonians provide a rigorous link between very accurate atomistic length scale ab initio methods and very efficient meso- and macro-scale continuum methods, such as the phase field method, for describing materials thermodynamics and kinetics. I will describe current progress in our development of an open source software package, CASM (A Clusters Approach to Statistical Mechanics). CASM automates the process for 1) formulating cluster expansion effective Hamiltonians based on the symmetry of the materials system, 2) parameterizing cluster expansion effective Hamiltonian coefficients from ab initio calculations, and 3) calculating continuum scale thermodynamic and kinetic properties, such as composition and strain-dependent free energies and diffusion coefficients, using Monte Carlo methods. Developed with support from the Center for PRedictive Structural Materials Science (PRISMS) at the University of Michigan, CASM provides an essential component for integrated computational materials engineering. As an example application, I will describe the use of CASM for studying the electronic, thermodynamic and kinetic properties of the Zr-O system [1]. Using an ab initio parameterized cluster expansion Hamiltonian and grand canonical Monte Carlo calculations we find evidence of an infinite sequence of 0-K ground-state ZrO_x suboxide phases consisting of unique stackings of empty, 1/3-filled, and 2/3-filled layers of oxygen in octahedral interstitial positions of the hexagonal close packed lattice. Using a k-space analysis we rigorously identify order-disorder transitions between the suboxide phases. We also identify the structure of a previously uncharacterized Zr-monoxide phase, with a structure related to δ -TiO. The Zr monoxide structure is equivalent to the high-pressure ω -Zr phase but has interstitial oxygen ordering. [1] B. Puchala and A. Van der Ven, Phys. Rev. B, 88, 094108 (2013).

Title: Acceptance Criteria for Structural Response to Impact and Blast Loading

Author(s): John Puryear, William Leboeuf, Matthew Kraemer, *ABS Consulting*.

Finite element analysis (FEA) is increasingly being used as a tool for the analysis and design of structures subjected to impact and blast loading. Various organizations have published guidance on how much deformation in response to impact and blast is acceptable. Such guidance typically proposes a limiting plastic strain, whether effective plastic strain or plastic strain along the principal axes. The difficulty for analysts is that the guidance available in the public domain is often incomplete, contradictory and lacks a consensus. For FEA to continue developing as a design tool, unified and consistent acceptance criteria for deformation must be developed. In this presentation, the authors will review published guidance on acceptance criteria for steel structures, as an example. Case studies illustrating how the criteria have been applied will be discussed. Finally, the authors will propose paths toward developing unified and consistent acceptance criteria for structural response to impact and blast. Examples of acceptance criteria from other types of impact and blast analysis, such as single-degree-of-freedom (SDOF), will be considered. SDOF acceptance criteria have been disseminated by the US Army Corps of Engineers Protective Design Center and the American Society of Civil Engineers. The success of these criteria can serve as a model for developing acceptance criteria for FEA.

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Title: An Embedded/Immersed Boundary Type Coupling of Overlapping Lagrangian and Eulerian/ALE Meshes

Author(s): Mike Puso, Ed Kokko, Ben Liu, Brian Simpkins, *LLNL*.

Methods for coupling superposed foreground and background meshes are useful for simplifying model development and providing solution strategies that can be more robust and flexible than standard ALE. Here, these coupling techniques are referred to as embedded mesh methods but have been also referred to in the literature as immersed boundary, fictitious domain etc. An embedded mesh approach using piece-wise Lagrange multipliers with pressure stabilization is applied to transient dynamics using the central difference scheme for the time discretization. By solving for the multipliers iteratively, it is shown that the resulting equations of motion are a stable linear system with a condition number independent of mesh size and the time integration of the scheme is provably stable with a critical time step computed from the un-constrained equations of motion. The extension for coupling Lagrange foreground meshes to multiple-material ALE type background meshes using a time splitting approach is also presented. The modifications for advection can avoid the “leaking” often associated with these methods. Example problems demonstrate convergence and applicability to a range of problems. In particular, the fluid-structure interaction examples focus on blast applications.

Title: Simulation Techniques for Porous Media Confined in Silo Geometry

Author(s): Abdul Qadir, Kashif Hussain, Aziz Altaf khuwaja, *Sukkur Inst.* .

Granular materials have vast applications both in industry and in daily life. They display quite interesting and exceptional properties different from the other known forms of matter. To investigate the complex properties of particulate materials, experimental, analytical and simulation techniques have been employed. In this paper the results of large-scale discrete element molecular dynamics (DEM) simulations in three dimensions are reported. It deals with the investigation of stress deflection due to various grain sizes. Moreover, the influence of coefficient of friction between granules and cylindrical walls on the mass measured at bottom of container i.e. apparent mass is thoroughly investigated. Principal Contribution to the Field: It is revealed that apparent mass varies linearly with the grain size. In addition to that, it is also found that the apparent mass variation is strongly dependent on bead diameter rather than the silo. The results reveal that conversion of vertical stresses into horizontal in silo is mainly due to the friction between the grain and system boundary. This minisymposium will serve as a platform to exchange ideas on novel computational techniques that increase the accuracy and/or the efficiency of simulations in connection with silo geometry. Referee: 1. Prof. Daniel I. Goldman Department of Physics Georgia Institute of Technology, USA daniel.goldman@physics.gatech.edu 2. Prof. Qingfan Shi Key Laboratory of Cluster Science, School of Physics, Beijing Institute of Technology, China qfshi123@bit.edu.cn

Title: Ideal Strength and Deformation Defects of Advanced Alloys

Author(s): Liang Qi, *U. Michigan.*

The ideal mechanical strength of a material is the maximum stress that its perfect crystal lattice can sustain before its failure by the elastic or phonon instability. Many aspects of mechanical behaviors for realistic materials are affected by the inherent features of the corresponding ideal strength properties. Here ab initio calculations are applied to investigate the ideal tensile and shear strength of several advanced alloys in both bcc and hcp lattices. The effects of alloying, temperature and mechanical loading conditions to ideal strength are systematically investigated, and the intrinsic electronic mechanisms to determine the ideal strength of these advanced alloys are evaluated. Furthermore, atomistic simulations and the constructions of continuum theories are performed in order to connect the ideal strength results to the properties of realistic deformation defects, such as dislocation core structures and crack tips. One example is how the ideal tensile and shear strengths of bcc refractory alloys (Mo, W) affect their dislocation nucleation under extreme strain conditions and the energetics/kinetics of dislocation core structures. This multiscale modeling scheme based on ideal strength calculations provides a guide for alloying processes aimed at increasing the plasticity of advanced alloys in low-symmetry (bcc and hcp) lattices.

Title: A Micromechanical Multi-Scale Damage-Friction Model for Initially Anisotropic Materials

Author(s): Mei Qi, Jean-Baptiste Colliat, *U. Lille1*; Albert Giraud, *U. Lorraine*; Jianfu Shao, *U. Lille1* .

This paper aims at modelling of coupling between damage evolution and frictional sliding in an initially anisotropic material with the help of numerical solution of Hill's tensor. Based on the homogenization method Mori-Tanaka, the damaged medium is characterized by an initially transversely isotropic solid matrix which is weakened by a family of penny-shaped microcracks. The interaction of sliding and damage evolution is addressed by performing a thermodynamic analysis and the linear Coulomb-type criterion. The friction criterion is formulated on the local scale with a back stress term applied onto microcracks. The back stress term which is involved by the free enthalpy plays the essential role in describing material hardening/softening. While the strain softening is increased by damage evolution, the stress hardening is cumulated by frictional shearing. Numerical examples are presented and compared with experimental data for a typical sedimentary rock.

Title: Integrated Multi-Scale Simulation Approach to Laser Material Interaction

Author(s): Dong Qian, Mohammad Karim, *UT Dallas*.

There is a continuing interest in exploring the fundamental mechanisms of laser material interaction in improving the mechanical performance of a wide range of manufacturing applications. The unique spatial and temporal profiles of the LSP pulse lead to microstructural evolutions in the materials that are not well-understood based on a single scale modeling approach. In this context, a multiscale simulation method that integrates the atomistic with continuum representations was established with a goal to link the relevant length scales. Efforts in applying the multiscale framework for laser processing of material will be presented. In particular, we will demonstrate the application of the so-called bridging scale approach [1, 2] and multiscale boundary conditions. Following a brief introduction of the bridging scale methodology, the detailed implementation on the modeling of laser pressure and material responses will be presented. In particular, we highlights the ability of the multiscale methodology in incorporating critical experimental observations and providing detailed answers on the link among the laser process parameters, coupon/parts configurations and material responses. References [1] G. J. Wagner and W. K. Liu, "Coupling of atomistic and continuum simulations using a bridging scale decomposition," *Journal of Computational Physics*, vol. 190, pp. 249-274, Sep 1 2003. [2] D. Qian, G. J. Wagner, and W. K. Liu, "A multiscale projection method for the analysis of carbon nanotubes," *Computer methods in applied mechanics and engineering*, vol. 193, pp. 1603-1632, 2004 2004.

Title: Towards Building Correspondence Rules Between Human and Pig Head Models for Traumatic Brain Injury

Author(s): Siddiq Qidwai, Amit Bagchi, *US Naval Rsch. Lab.*; Nithyanand Kota, *Leidos Corp.*.

Many parallel courses of study are being attempted to understand the complexity of the dynamic events associated with blast-induced traumatic brain injury (TBI). These include field testing of surrogate physical models, cadavers, and animals; laboratory experimentation on brain tissue and cell cultures; and computational modeling and simulation of the human head under impact scenarios, based on the finite element method. In order to create a cohesive and comprehensive understanding of TBI, however, one needs to be able to correlate the data obtained from these disparate approaches. In this regard, a framework is being developed in this study to develop TBI scaling rules between human head and pig head computational models. Both types of head models are obtained from magnetic resonance imaging (MRI) scans, which were digitized into voxels and then converted into very refined finite element meshes. Extensive image segmentation and processing, and manual intervention during image-to-voxel transformation made it possible to include all major components of the heads with high resolution. The human model is based on a 50th percentile Caucasian male of 26 years age, whereas the pig head model, including its upper torso, is based on a Yucatan mini-pig of 26.5 kg mass. The component material behaviors are defined with appropriate constitutive functional forms as dictated by the latest low-to-high rate data available in the literature. Finally, the human head model is validated against four well-known experimental studies related to the automotive industry, whereas the pig head and torso model is validated against blast tube injury response data obtained elsewhere. In this sense, the human head model can be directly related to the live pig data for specific impact scenarios. The comparison is made in terms of predicted regions and extent of injury. Multiple mechanical variables have been used to describe the occurrence of brain injury in impact modeling of the human head. The variables that best described injury in the pig model during the validation process are chosen for continued use. Based on this choice, initial results show that under the same blast impact the pig model show relatively less injury compared to the human head model. This may be attributed to the thicker skull of the pig. As the database is continually built based on more simulations, it is expected that a more quantitative correlation between the human head and pig head will soon be determined for blast-induced TBI.

Title: Numerical Simulations of Granular Behavior in Mining Comminution

Author(s): Xiangjun Qiu, *Metso Minerals*.

Numerical simulation methods such as CFD and DEM have been widely employed as tools to model granular media behavior. One of their applications is in the area of comminution in mining industry. But many times, the common numerical simulations cannot achieve the goals expected due to scale limitation. This presentation addresses the roles and limitations of various numerical simulation methods in the area of comminution. It is proposed that the main application domain for comminution can be divided into nine subdomains based on the classification of scales of granule size and bulk density. In each of subdomain, some specific modifications and/or algorithms are required in order for the numerical methods to play the role. As examples, two extreme models of comminution devices will be discussed. One is cone crusher which features medium solid fraction and coarse particle size. The other is high pressure grinding roll which features wide ranges of distributions of solid fraction and particle size.

Title: Discussion on Structural Inelastic Analysis Using the Force Analogy Method

Author(s): Jiting Qu, Zhongwen Shu, Tingwei Jiang, *Dalian U. Tech.*

Structure responds inelastic domain under a major earthquake, and this manifests such as inelastic extensions in braces, plastic rotations in beams and yield of isolated forms etc. Current inelastic analysis is to extend the well-established knowledge gained from elastic analysis by changing structural stiffness, mostly been done with strain-hardening materials while others remain difficult. Inelastic structures are dynamic stable under dynamic loadings with kinds of solutions, for instance, Newark- β method, Wilson- θ method and state space approach which is widely adopted as the application of computer. However, for complex structure with large matrix, state space method is very time consuming and costly, bringing about inaccurate results. Considering about these, a new algorithm using only initial stiffness—termed the force analogy method (FAM) is proposed, with the main concept of inelastic deformation firstly presented by Lin in 1968. One advantage of FAM is the dynamic stability and the other is stress would be determined once strain is confirmed, and inelastic deformation at a particular location is defined as a degree of freedom, which would simplify the analysis. In this paper, the improved theory of FAM is expounded and two questions are discussed firstly. (1) The initial stiffness is utilized when solving the plastic variable, such as the inelastic moment. The postyield stiffness (EI) is smaller than the initial stiffness according to the fundamental, so it will inevitably lead to the deviation of the results when use the initial stiffness to calculate the inelastic moment. (2) The relationship between inelastic rotation and inelastic displacement can be obtained by the fundamental equation. It is assumed that the postyield stiffness are K' and K_p' respectively. The ratio of K_p' and K' is a constant C at the same deformation condition. It can be derived that the ratio of K_p and K is also a constant. Secondly, by comparing two kinds of arrangement forms based on plastic rotational hinge, the reasonable arrangement form is found which was applied to nonlinear dynamic analysis of structure with viscous damper finally. Numerical simulation results indicate that the effectiveness of viscous damper and differences of local energy dissipation.

Title: Deconvolution-Based Nonlinear Filtering for Incompressible Flows at Moderately Large Reynolds Numbers

Author(s): Luca Bertagna, *Florida State U.*; Annalisa Quaini, *U. Houston*; Alessandro Veneziani, *Emory U.*

We consider a Leray model with a deconvolution-based indicator function for the simulation of incompressible fluid flow at moderately large Reynolds number (in the range of few thousand) with under-resolved meshes. For the implementation of the model, we adopt a three-step algorithm called evolve-filter-relax (EFR) that requires the solution of a Navier-Stokes problem, the solution of a Stokes-like problem to filter the Navier-Stokes velocity field, and a final relaxation step. We take advantage of a reformulation of the EFR algorithm as an operator splitting method to analyze the impact of the filter on the final solution vs a direct simulation of the Navier-Stokes equations. In addition, we provide some direction for tuning the parameters involved in the model based on physical and numerical arguments. Our approach is validated against experimental data for fluid flow in an idealized medical device (consisting of a conical convergent, a narrow throat, and a sudden expansion, as recommended by the Food and Drug Administration). Numerical results are in good quantitative agreement with the measured axial components of the velocity and pressures for two different flow rates corresponding to turbulent regimes, even for meshes with a mesh size more than 40 times larger than the smallest turbulent scale. Through a large set of numerical experiments, we perform a preliminary sensitivity analysis of the computed solution to the parameters involved in the model.

Title: Hybrid-Mixed, Finite-Element Method on Quadrilateral Meshes

Author(s): Thiago Quinelato, Abimael Loula, *Nat'l. Lab. Scientific Computing*; Maicon Correa, *U. Campinas*.

Solutions of classical $H(\text{div})$ -stable finite element spaces, such as Raviart-Thomas (RT), Brezzi-Douglas-Marini (BDM) and Brezzi-Douglas-Fortin-Marini (BDFM), may suffer a decrease in the convergence rates on meshes with distorted quadrilaterals when compared to those obtained on meshes of parallelograms. Arnold, Boffi and Falk (2005) presented a necessary and sufficient condition that a pair of $H(\text{div})$ -stable spaces must satisfy in order to exhibit optimal rates of convergence in distorted meshes. A new family of spaces that satisfy that condition was also proposed in their work. In this work we propose a novel stabilized hybrid mixed finite element formulation for the Poisson problem combining the finite element spaces introduced in Arnold, Boffi and Falk (2005) with a stabilization technique based on the addition of Galerkin and least-squares residuals of the equations in the interior of the elements. Numerical results evidence that this strategy allows the attainment of high order approximations in $H(\text{div})$ on arbitrary quadrilaterals while enabling a flexible choice for the finite dimension spaces.

Title: Influence of Arterial Wall Properties on Simulation of Pulse Wave Propagation in a 1D Network Model

Author(s): Muhammad Qureshi, Christina Battista, *NCSU*.

Computationally efficient 1D fluid dynamics models are useful tools for understanding the fluid-structure interaction and flow dynamics within the arterial network [2]. Basic building blocks of these models consist three types of equations, two equations ensuring conservation of mass and momentum and a constitutive equation relating blood pressure and arterial cross-sectional area, as well as the set of boundary conditions at the network inflow, outflow and junctions. The study of transient properties of the pulse wave via such models, including the type and arrival times of reflected waves, provides us useful insight into the nature of fluid-structural interaction in the arteries. The interaction of incident and reflected waves determines the shape of pressure profile at the proximal arterial locations. The shape of pressure wave is not only an important physiological marker of cardiac events but also carry useful information about the architecture of arterial network, such as types of junctions, and wall properties. It has been shown [1] that the prediction of pulse pressure in such models is greatly influenced by the elastic and viscoelastic properties of the arterial wall, included via the constitutive wall model. Specifically, the elastic component of the wall models in an arterial network model has shown to impact the transient times of incident and reflected waves due to change in the pulse wave velocity (PWV) [3]. In this talk we will shed light on the influence of elastic and viscoelastic properties on the pulse wave propagation by investigating the PWV and patterns of incident and reflected pressure wave along an arterial lumen, isolated and within a network model. Using some example results, we will illustrate how wall viscosity influence the compressive nature of initially propagated forward pressure wave in the systole and consequently on its reflected component arriving later in the cardiac cycle. We will also show results of how different wall models and associated parameter values affect the ability of 1D models to assess the techniques to estimate the PWV, which use the in vivo hemodynamic signals such as the blood pressure and velocity. [1] C. Battista, et al. *J Mech Med Biol*, 2015. [2] F.N. van de Vosse, N. Stergiopulos. *Annu Rev Fluid Mech*, 43:467-499, 2011. [3] M. Umar Qureshi, N.A. Hill. *J of Math Biol*, DOI: 10.1007/s00285-015-0867-2, 2015.

Title: Remeshing Techniques for 2D Models Using a Smoothed Representation of Recovered Boundaries

Author(s): Harish Radhakrishnan, Jin Wang, Siddhartha Mukherjee, *ANSYS Inc.*

Finite element modeling of elastomeric components such as seals which undergo severe geometric distortion are often impossible without remeshing. During remeshing an often used technique to preserve the geometry of the remeshed domain is to retain the nodal locations on the boundary. This imposes constraints on the quality of the regenerated mesh. In this work we discuss a developed technique which permits the generation of the new mesh on the smoothed representation of the recovered boundary from facets of deformed mesh. This allows greater flexibility in creation of the new mesh. To ensure that the boundaries of the old and new mesh are consistent, we perform correction to project the boundary nodes of the new mesh to lie on the boundary of the old mesh. The technique is robust and is capable of handling self contacts with no special treatment. Further all kinematic boundary conditions, locations of applied external loads and interaction model definitions are retained maintaining consistency between the old and new mesh. We demonstrate the viability of method with multiple examples in the 2d axis symmetric domain and discuss the possibility of automating the approach.

Title: A Non-Isothermal Phase-Field Model for Damage in Biphase Brittle Materials

Author(s): Markus Radszuweit, Christiane Kraus, *WIAS-Berlin*.

Modeling failure in complex solid materials requires consideration of inhomogeneous elastic, toughness and thermal properties. Phase field models have shown to be a suitable tool to approach such multi-phase and multi-physics problems on a macroscopic level. They provide an elegant way to deal with discontinuities without tracking complicated crack surfaces (or paths in two dimensions). An evolution equation is presented that is derived from a variational ansatz for a given free energy and a dissipative pseudo-potential based on Ref. [1]. Constraints that enforce irreversibility of damage evolution are used as in [2]. Within this framework a Griffith-like criterion is fulfilled. Depending on the choice of the free energy this model is capable of describing smooth damage as a homogenized field of microcracks, as well as cracks with sharp interfaces. Based on recent work [3] that introduced a coupling to a two-phase model for spinodal decomposition (Cahn-Larché system with damage) a further extension incorporating thermal effects is shown. This is of particular relevance, since different thermal expansion is well known to cause failure when temperature varies significantly during operation or manufacturing of a structure. Finite Element simulations in two dimensions are used to investigate solutions of the presented model, in particular the influence of inhomogeneities on the crack path. The main challenges to overcome in numerical simulations are the presence of inequality constraints resulting from the irreversibility of damage evolution and the relevance of multiple spatiotemporal scales involved in crack propagation. Adaptive re-meshing and time step control is used to deal with the latter. References: [1] G.A. Francfort, and J.J. Marigo. Revisiting brittle fracture as an energy minimization problem. *J. Mech. Phys. Solids* 46 (1998): 1319-1342 [2] M. Frémond, and B. Nedjar. Damage, gradient and principle of virtual power. *Int. J. Solid structures* 33 (1996): 1083-1103. [3] C. Heinemann, and C. Kraus. Existence of Weak Solutions for Cahn-Hilliard Systems Coupled with Elasticity and Damage. *Adv. Math. Sci. Appl.* 21 (2011): 321-359

Title: Geometric Partitioning Sensitivity Analysis

Author(s): Shad Kirmani, Jeonghyung Park, Padma Raghavan, *Penn State U.*

We consider the class of geometric schemes for partitioning graphs, which have their vertices, embedded in 2D/3D space. These parallel schemes typically show better performance on larger number of processors, compared to other types of parallel partitioning schemes such as algebraic and spectral graph partitioning. We specifically consider Recursive Coordinate Bisection and its implementation in Zoltan and ScalaPart implementation of Geometric Mesh Partitioning. The problem of geometric graph partitioning arises in many applications such as iterative schemes for finite element methods, circuit design, etc. The quality of partitions computed by a graph partitioning scheme is better if number of edges crossing the partitions is low. Moreover, the partitions should be robust to perturbation in vertex coordinates, bad mesh quality meshes and approximate embedding. To achieve a high quality partition of an embedded graph, we can either spend time on computing a good embedding or working on more complex partitioning algorithms for embedded graphs. Ideally we would like the geometric partitioning scheme to compute high quality partitions on graphs with only approximate embeddings. Understanding the tradeoffs will help in better usage of the existing geometric partitioning algorithms and also in the development of better geometric partitioning algorithms. In this paper we study a very popular geometric partitioning scheme, Recursive Coordinate Bisection, from the Zoltan package and the recently developed parallel geometric scheme, ScalaPart, based on multiple 'sphere' cuts. We find that the number of tries and refinement affects both ScalaPart and RCB respectively. We also find that ScalaPart is more robust in terms of partition quality to perturbation of coordinates, mesh quality and approximate graph embedding. ScalaPart is slower than RCB but shows better speedup unto 32 cores.

Title: A Coupled 3D Four-Constituent Tumor Growth Model Based on Continuum Mixture Theory

Author(s): Mohammad Rahman, Yusheng Feng, *UTSA*; Jun Zhou, *UT Austin*.

The growth of the tumor is a complex process involving various mechanical- and biochemical-induced events at different length scales. To formulate the avascular three-dimensional (3D) tumor growth problem in the macroscopic scale, we propose a continuous model where the tissue is represented as a mixture of four constituents consisting of tumor tissue, healthy tissue, water and nutrient (oxygen) dissolved in the water. The governing equations are developed based on both mass and momentum conservation laws. The constitutive laws are derived from the tumor growth process. Specifically, both tissue anisotropy (transverse isotropy) and neo-Hookean tissue behavior are accounted for in the constitutive relationships. The momentum exchange among the constituents is modeled based on the Coleman-Noll procedure by employing the entropy inequality [1, 2]. The growth factors in the computational model are calibrated using experimental results from the literature [3]. The simulation results resemble the amorphous tumor morphology and show the absence of nutrient at the core, which will eventually trigger the necrosis. The results also show the velocity, pressure and stress distribution in both tumor and healthy tissue domains revealing their effects in the growth process. This model can help us better understand the tumor growth process. It can also potentially be used as a patient-specific tumor growth model for treatment planning and prognosis. References: [1] Coleman, B. D., and Noll, W. (1963). The thermodynamics of elastic materials with heat conduction and viscosity. *Archive for Rational Mechanics and Analysis*, 13(1), 167-178. [2] Cimmelli, V. A., Sellitto, A., and Triani, V. (2010). A generalized Coleman–Noll procedure for the exploitation of the entropy principle. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* (Vol. 466, No. 2115, pp. 911-925). The Royal Society. [3] Bao, A., Phillips, W. T., Goins, B., McGuff, H. S., Zheng, X., Woolley, F. R., Natarajan, M., Santoyo, C., Miller, F. R., and Otto, R. A. (2006). Setup and characterization of a human head and neck squamous cell carcinoma xenograft model in nude rats. *Otolaryngology--Head and Neck Surgery*, 135(6), 853-857.

Title: Numerical Framework for Mesoscale Simulation on Heterogeneous Energetic Materials

Author(s): H.S. Udaykumar, Nirmal Kumar Rai, *U. Iowa.*

Heterogeneous energetic materials have complicated microstructure and contain various forms of heterogeneities such as pores, micro-cracks, binders, energetic crystals etc. It is widely accepted that the presence of these heterogeneities can affect the ignition threshold of these materials. Shock interaction with the heterogeneities leads to the formation of local heated regions known as hot spots. Depending on the hot spot temperature, reaction triggers and grows eventually leading to ignition and formation of detonation waves. Hot spot formation can take place through various physical phenomenon such as pore collapse[1], formation of shear bands leading to local heated regions due to viscoplastic work, inter-granular friction in HMX crystals, shock heating of HMX crystals and binder etc. In order to understand different mechanisms for the formation of hot spots and to establish ignition threshold criterion for energetic materials, a robust numerical framework is desired which can capture the appropriate physics. In the present work, a numerical framework has been developed to perform shock initiation studies on heterogeneous energetic materials such as plastic bonded explosives (PBX) and pressed explosives using mesoscale simulations. The microstructure geometry of these materials has been modeled by employing sophisticated image processing algorithms on XCMT and SEM images. The image processing framework is incorporated in a massively parallel Eulerian code SCIMITAR3D[2] for the mesoscale simulations. The chemical decomposition of HMX has been modeled using Henson-Smilowitz multi-step mechanism. The validation of the numerical framework has been established by comparing with the experimental results. 1. Kapahi, A. and H. Udaykumar, Dynamics of void collapse in shocked energetic materials: physics of void-void interactions. *Shock Waves*, 2013. 23(6): p. 537-558. 2. Kapahi, A., S. Sambasivan, and H. Udaykumar, A Three-Dimensional Sharp Interface Cartesian Grid Method for Solving High Speed Multi-Material Impact, Penetration and Fragmentation Problems. *Journal of Computational Physics*, 2013.

Title: Isogeometric Modeling and Discretization of Contact Problems

Author(s): Martina Matzen, Ekkehard Ramm, Manfred Bischoff, *U. Stuttgart.*

The higher inter-element continuity of NURBS functions is a key property of the Isogeometric Analysis (IGA). The applied IGA contact formulation utilizes a Lagrange Multiplier Method avoiding numerical instabilities often present in a Node-To-Segment (NTS) approach. The present Point-To-Segment (PTS) formulation places collocation points directly on the contact surface [1]. However the patch test is still not satisfied. This problem can be remedied if the contact integral is not collocated but numerically integrated applying the Segment-To-Segment (STS) contact formulation [2]. In this case the quadrature points play the role of evaluation points of the contact equation. PTS and STS differ only in the underlying Lagrange multiplier field, in number, location and weights of these points, as well as in their efficiency. In the present study the PTS formulation is equipped with features of the STS version, namely also introducing a field for the Lagrange multiplier, but still collocating the contact integral, for example at Greville or Botella points. Weights are assigned to the expressions at these points reflecting the corresponding influence regions. Numerical examples show the same accuracy in displacements as the original PTS algorithm; concerning the result of the Lagrange Multiplier contact stresses instead of contact forces are obtained. For complex examples including friction, results of the PTS+ (with additional weights) compared to the ones of the STS approach are of the same quality, but require considerable less computational time. The extension to dynamic problems applies a Newmark algorithm avoiding instabilities of the integrator by splitting the acceleration in a contact and non-contact part [3] and regularizing the contact force by mass relocation. REFERENCES [1] M.E. Matzen, T. Cichosz and M. Bischoff, "A point-to segment contact formulation for isogeometric, NURBS based finite elements" Derivation of thin plate bending elements with one degree of freedom per node", *Comput. Methods Appl. Mech. Engrg.*, Vol. 255, pp. 27-39, (2013). [2] I. Temizer, P. Wriggers and T.H.R Hughes, "Contact treatment in isogeometric analysis with NURBS", *Comput. Methods Appl. Mech. Engrg.*, Vol. 200, pp. 1100-1112, (2011). [3] T. Cichosz, "Stabile und konsistente Kontaktmodellierung in Raum und Zeit", Report No. 58, Institute for Structural Mechanics, University of Stuttgart, PhD thesis, 2012.

Title: A Study of Modeling Error in the Computational Homogenization of Complex Microstructures

Author(s): James Ramsey, *Army Rsch. Lab.*

As exemplars of representative volume elements (RVEs) for which numerical estimation of elastic properties may be difficult or unreliable, three-dimensional images of simulated microstructures of cement at an early stage of curing have been utilized. A massively parallel finite element implementation of asymptotic expansion homogenization (AEH) has been used to determine elastic properties of not only the early-age cement microstructures themselves, but other microstructures whose properties can be more reliably estimated, namely a copper polycrystal and a unidirectional composite. Several images of cement RVEs, with resolutions varying from 100x100x100 to 1000x1000x1000, are generated via CEMHYD3D, cement hydration simulation software from NIST (National Institute of Standards and Technology). Other images of cement RVEs are coarsened versions of the 800x800x800 and 1000x1000x1000 images from CEMHYD3D. At least one homogenization calculation has been done for each cement RVE, wherein the finite element mesh for the calculation has been generated using one element per voxel of the RVE image. In addition, for lower-resolution RVE images, additional homogenization calculations have been done in order to determine convergence rates of calculated elastic properties as the initial finite element mesh is further refined, and elastic properties as mesh resolution approaches infinity have been estimated via curve fitting. Convergence rates (i.e. effectively the exponents of the reciprocal element width) for cement RVEs range from about 1.0 to 1.2, slightly poorer than that for the polycrystal, about 1.3, and much poorer compared to those of the unidirectional composite, which range from about 1.5 to 2.0. Of more concern, though, is that for the cement RVE images, the finite element mesh produced by the common practice of using one finite element per voxel yields unreliable elastic stiffnesses that apparently overestimate the estimated infinite-resolution values by factors of 250-600%, a problem that does not occur for even the coarsest meshes of the unidirectional composite and polycrystal (with about 2500 and 15,000 elements, respectively), and this, combined with the poor convergence, means that even a calculated elastic stiffness for a mesh refined to a resolution of 900x900x900 elements may overestimate the estimated infinite-resolution value by 150%. Furthermore, the estimated infinite-resolution values for apparently similar microstructures can vary by factors of about 140-270%, indicating additional uncertainties in the determination of elastic properties for the cement RVEs. Reasons for these difficulties, what may be done to ameliorate them, and their implications for non-cement microstructures, are to be discussed.

Title: The Finite Cell Method: Basic Principles and Recent Progress

Author(s): Ernst Rank, Tino Bog, Laszlo Kudela, Stefan Kollmannsberger, Nils Zander, *Tech. U. München.*

The finite cell method (FCM) [1] is a combination of a fictitious domain approach with finite elements of high order. The physical domain is embedded into an easy to mesh bigger computational domain. Finite cell meshes are then generated ignoring boundaries of the physical domain and result in rectangular 'cells' as support for the higher order shape functions. The geometry of the problem is only considered during the integration of the cell matrices. To this end an indicator function is introduced being equal to 1 inside the physical domain. Outside it is set (in order to avoid conditioning problems) to a very small value. The contribution of the fictitious domain is thus penalized, shifting the effort of meshing towards the numerical integration of the cell matrices. Combining these ingredients, an exponential rate of convergence can be observed for smooth problems, when performing a p-extension [2]. Since the quality and efficiency of the finite cell approximation strongly depends on the numerical integration scheme, this presentation will first discuss a new algorithmic subdivision approach, extending the conventional octree-based integration with the ability of resolving 'kinks' or corners of the physical domain. In combination with the blending function method, this algorithm yields a nearly exact decomposition of the cut cells. Our approach is able to resolve close-to-degenerate cases, but remains algorithmically simple at the same time. Several further recent developments of the FCM will be discussed. A new two- and three-dimensional hierarchical refinement strategy yields exponential rate of convergence in energy norm even for singular problems [3], and its simple algorithmic structure allows an easy extension to transient problems with local refinement and de-refinement. Finally, a re-interpretation of the fictitious domain in the sense of a 'third material' opens the way for a modified contact formulation without the necessity of contact search. [1] Düster, A.; Parvizian, J.; Yang, Z.; and Rank, E. (2008). The finite cell method for three-dimensional problems of solid mechanics. *Computer Methods in Applied Mechanics and Engineering*, 197:3768–3782. [2] Dauge, M.; Düster, A.; Rank, E. (2015). Theoretical and numerical investigation of the finite cell method, *Journal of Scientific Computing*, accepted, #JOMP-D-14-00097R1 [3] Zander, N.; Bog, T.; Kollmannsberger, S.; Schillinger, D.; Rank, E (2015). Multi-Level hp-Adaptivity: High-Order Mesh Adaptivity without the Difficulties of Constraining Hanging Nodes, *Computational Mechanics*, accepted, DOI: 10.1007/s00466-014-1118-x

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

Title: A Hybrid ALE-CDFEM Approach to Modeling Foaming in Punch Molds

Author(s): Rekha Rao, David Noble, Scott Roberts, *Sandia Nat'l. Lab.*; James Tinsley, *Honeywell Nat'l. Security Campus*.

Punch molds are used to create thin, high density polymeric foam parts. In this process, foam precursor is poured into the bottom of a mold and then an insert is then placed in the mold to create the foam part. The shape of the mold and the insert is complex, requiring a full three-dimensional analysis. The process involves multiple time-scales with a fast insertion of the insert causing the foam precursor to splash up while it is still a low viscosity fluid. Once the insert is in place, the foam reactions begin causing the material to simultaneously polymerize and generate gas. The reaction time-scale is much slower than the initial splashing flows. The final result of the process creates a thin walled foam solid. Modeling the punch molding process is quite complex and requires a coupled approach. The geometry evolves with the insertion of the inner mold and this effect is captured using an arbitrary-Lagrangian-Eulerian (ALE) approach to move the mesh. The foam expansion is tracked using a conformal decomposition finite element method (CDFEM) to determine the location of the free surface as it evolves through splashing and foaming. The CDFEM has to interact with the background moving mesh and still be conservative. The method is demonstrated on a simple two-dimensional punch molding problem. We will also discuss extensions to three-dimensions. 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.

Title: Polyhedral FEM: Computational-Geometry Aspects

Author(s): Mark Rashid, *UC Davis*.

Freedom from the constraints associated with isoparametric mesh generation is usually cited as the main advantage of polyhedral finite elements. Indeed, an absence of strict topological and geometric requirements on the individual elements would seem to open up exciting possibilities with regard to automation of the geometry-to-analysis process. However, realizing the full potential of polyhedral finite elements involves some significant challenges. In this regard, two interconnected elements are evident: 1) robustness of the element formulation itself, and 2) robustness and degree of automation of the polyhedral mesh-generation capability. With regard to the latter, the polyhedral mesher should ideally be capable of automatically discretizing an arbitrary 3D problem domain given only an explicit boundary representation of the domain, along with minimal user directives related to target mesh density and its spatial variation. This meshing process should, without human intervention, reliably produce valid polyhedral meshes whose every element conforms to whatever restrictions the element formulation imposes. The polyhedral element formulation, on the other hand, should be as free of geometric and topological restrictions as possible, as these inevitably diminish the prospects for truly reliable automated meshing. The elements of an integrated solid modeling, meshing, and polyhedral-FEM-based approximation system that achieves these objectives will be presented. The approximation scheme -- the so-called Partitioned Element Method (PEM) -- will be summarized, followed by an examination of the computational-geometry aspects of polyhedral-FEM-based simulation. Polyhedral auto-meshing begins with a solid model defined by an explicit, facetized boundary representation (b-rep) of the problem domain. For the b-rep to be suitable for use as input to a polyhedral meshing algorithm, it should possess certain properties not guaranteed by typical CAD systems, such as exact topological correctness, flat polygonal facets, and freedom from arbitrarily small polytopes. The subsequent meshing phase should exhibit corresponding properties. Both of these operations -- solid-model creation and polyhedral meshing -- rely on Boolean geometric operations whose algorithms are dominated by tolerance issues and degeneracy resolution. A new approach to these issues, "tolerance-aware geometric computation," will be described which affords control over the minimum feature size (e.g. elements, facets) in the output, while guaranteeing topological correctness. The tolerance-awareness concept is also applicable to Voronoi partitioning of 3D space, which is an important element of the PEM formulation. Illustrative problems and work flows will also be presented.

Title: CRKSPH: A Conservative Reproducing Kernel Smoothed Particle Hydrodynamics Scheme

Author(s): Cody Raskin, LLNL.

Suitable modifications to the SPH interpolation scheme first suggested by Liu et al. (1995) allow for the exact reproduction of constant, linear, or higher order fields, and these modifications are commonly referred to as reproducing kernel methods (RPKM). However, efforts in this realm have run into difficulties maintaining conservation of momentum when the kernel functions are no longer symmetric. We demonstrate a version of smoothed particle hydrodynamics that employs a first-order consistent smoothing function that exactly reproduces linear fields, building on RPKMs, while also maintaining momentum conservation. This scheme confers all of the benefits of traditional particle methods, such as Galilean invariance and natural conservation of momentum, while also eliminating some of their shortcomings, such as overly aggressive artificial viscosity and their inability to reproduce linear fields. We employ a simple fix to the momentum equation first derived for moving least-squares SPH methods (Dilts 1999) to our reproducing kernels that restores conservation. We also show how the reproducing kernel method's more accurate approximation of the velocity gradient allows for a much more conservative form of artificial viscosity, which hitherto fore has been a barrier to particle codes being employed for problems featuring fluid instabilities such as the Kelvin-Helmholtz instability.

Title: Convergence and Noise Statistics in Multiplicative Regularization

Author(s): Orsola Rath Spivack, Yujun Qiao, *U. Cambridge.*

In the treatment of noisy inverse problems few results are available concerning the qualitative and quantitative effects of the statistical distribution of the noise. We consider the case when the operator to be inverted is a convolution, found in many problems including image deblurring and inverse scattering. Common schemes for the solution of such inverse problems involve the minimisation of a cost functional composed of a data fidelity term, plus a regularising term ('additive regularisation', such as Tikhonov regularisation). Additive regularisation always requires also a method for choosing one (or more) regularisation parameters, and this is usually expensive numerically and highly nontrivial when the inverse problem is nonlinear. In the nonlinear case the problem will also need to be linearised at some stage in order to ensure convexity, and few results are known for the error involved in the iterative minimisation of the cost functional. A more recent type of regularisation involves a cost functional which is the product of the data fidelity term and a regularising term ('multiplicative regularisation', [Abubakar et al, IEEE Trans. Image Processing, 2004, 1524-1532]). It implements an algorithm that automatically chooses the regularisation parameter at each iteration, as well as - at least in principle - ensuring the convexity of the cost functional in all cases. This method has been shown to give good results in applications, but limited error analysis is available. We investigate the convergence and the dependence of the error in multiplicative regularisation on the type of noise distribution and for different noise levels, and compare with the behaviour in the case when additive regularisation is used. It is found that solutions using multiplicative regularisation are typically better than those obtained with additive regularisation, but the method is usually more expensive numerically. Statistical analysis using Monte Carlo and theoretical methods gives further insight into the behaviour.

Title: Investigation of Mechanical Parameters Role on the Morphogenesis of Cortical Folding

Author(s): Mir Jalil Razavi, Ryan Romeo, Tianming Liu, Xianqiao Wang, *U. Georgia*; Tuo Zhang, *Northwestern Polytech. U.*

Convoluting cortical folding, characterized by convex gyri and concave sulci, has an intrinsic relationship to the brain's functional organization. Understanding the mechanism of convolution patterns can provide useful insight into normal and pathological brain functioning. However, despite decades of speculation and endeavors the underlying mechanism of the folding process remains poorly understood. In this work, cortical folding phenomenon is interpreted both analytically and computationally, and in some cases the findings are validated by experimental observations. In the analytical part a soft structure with outer cortex and inner core is modeled as the living human brain so as to imitate the growth, and both deformation and stress fields inside the brain are derived and analyzed. Analytical interpretations for both isotropic and tangential growth of the brain model provide preliminary insight into critical growth ratios for instability and crease formation but it fails to predict the evolution of cortical complex convolution after the critical point. In the computational part, non-linear finite element models based on finite growth are employed to present crease formation and secondary morphological folds of the growing brain. Different initial geometry based on experimental literature has been considered and evaluated after growth, instability and post-perturbation. Results demonstrate that, dependent on the cortex-to-core growth ratio for differential growth of the brain model, compressive residual stresses trigger instability and cause crease formation. Initial geometry of model and initial thickness and material properties of the outer cortex relative to the inner core have a great effect on the morphological patterns of the growing brain. After instability, in the growing model, a thick cortex leads to the formation of fewer gyri and sulci (low gyrification index) which is consistent with Lissencephaly malformation in the developing brain, while a thin cortex leads to a high number of shallow gyri which is referred to as Polymicrogyria abnormality. Extended models showed that in addition to the thickness of cortex, the shear modulus ratio between the cortex and core may have the crucial effect on the morphological evolution of the growing brain. A higher stiffness of the cortex causes the growing model to prefer to wrinkle instead of creasing. Simulation results suggest that cortex/core differential growth assumption may only produce unregulated convolution while consistent and reproducible convolution patterns on cerebral cortex are regulated by regional growth heterogeneity which is controlled by regional differentiation of RGCs in the early stage of development in the fetal brain.

Title: Hi2Mod: High-Order Isogeometric Hierarchical Model Reduction of Elliptic Problems in Curved Domains

Author(s): Simona Perotto, Paolo Rusconi, *Politecnico di Milano*; Alessandro Reali, *U. degli Studi di Pavia*; Alessandro Veneziani, *Emory U.*

Many applications in engineering and scientific computing demand surrogate models that are expected to be computationally effective, yet reliable from a modeling viewpoint. In this presentation we focus on surrogate models devised to reduce physical problems characterized by a leading direction enriched by locally significant transverse dynamics. A relevant example is the modeling of the blood flow in arteries. Hierarchical Model (HiMod) reduction obtains surrogate models by resorting to a different discretization of the full problem with respect to the main and the transverse dynamics. In its original formulation, the mainstream is tackled by affine finite elements while spectral approximation solves the transverse directions. The rationale is that relatively few modes are enough to capture the transverse dynamics of interest with an overall reduction of computational costs. Numerical results show that the approach is versatile and effective, possibly coupled with modal/nodal adaptivity in the transverse/axial direction, respectively. The choice of affine elements is however limiting the range of applications that can be reliably solved. In particular, non rectilinear centerlines for the mainstream – that occur in fluid dynamics as well as structural dynamics - are approximated by piecewise linear functions, with an expected negative impact on the accuracy. Goal of this talk is to present a new version of the HiMod approach to enhance the standard performances for curved domains. In particular, we replace the finite element discretization along the mainstream with an isogeometric approximation. This new combination of discretization techniques in correspondence with primal and secondary directions yields the so-called Hi2Mod reduction. Hi2Mod provides a perfect computational synergy since the IsoGeometric Analysis (IGA) higher-regularity allows to reduce the number of axial degrees of freedom and eventually the global computational burden; in addition, the IGA intrinsic formulation allows a simpler and more effective geometrical modeling when curved domains are considered. In particular, centerlines are naturally obtained as splines or NURBS as it happens in practical (bio)engineering applications. We formalize this new approach on a standard scalar advection-diffusion-reaction problem, by numerically investigating the advantages of Hi2Mod formulation in terms of convergence and computational costs. In more detail, we compare the new scheme with the standard HiMod approach tailored on curved domains as well as with an isoparametric reformulation of the HiMod procedure. Possible future extensions of the Hi2Mod approach to more realistic fluid dynamic problems will be finally discussed, with a particular focus on hemodynamics.

Title: Natural Vorticity Boundary Conditions on Solid Walls and Application to Velocity-Vorticity Methods for Navier-Stokes

Author(s): Leo Rebholz, *Clemson U.*

We derive boundary conditions for the vorticity equation with solid wall boundaries. The formulation uses a Dirichlet condition for the normal component of vorticity, and Neumann type conditions for the tangential components. In a Galerkin (integral) formulation the tangential condition is natural, i.e. it is enforced by a right-hand side functional and does not impose a boundary constraint on trial and test spaces. The functional involves the pressure variable, and we discuss several velocity-vorticity formulations where the proposed condition is appropriate. Several numerical experiments are given that illustrate the validity of the approach.

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

Title: OOF: A Materials Science Focused Finite Element System

Author(s): Andrew Reid, Stephen Langer, Gunay Dogan, Shahriyar Keshavarz, *NIST*; Yannick Congo, *NIST/ICMA*.

An important component of modern materials design or high-throughput characterization efforts is rapid and flexible assessment of the behavior of model systems which encompass both spatial inhomogeneity, due to the presence of nontrivial microstructure, and the presence of multiple interacting fields, such as strain and temperature. The Object-Oriented Finite Element (OOF) software has been developed at the National Institute of Standards and Technology to provide a tool for materials scientists facing these kinds of modeling problems. The software takes as inputs the constitutive laws for the individual phases which make up the model system, and an image of the microstructure, which may come from either microscopy of a system under assessment, or from prior modeling steps or design iterations. It encapsulates powerful mathematical methods, making them available to materials scientists who are not themselves experts in finite-element modeling or numerical analysis, and allows these users to build high-quality meshes whose boundaries match the material boundaries in the model microstructure, while using an economical number of elements. Users can then vary the boundary conditions for the various fields, conducting virtual experiments to assess the effective properties of the systems, or conducting parametric analyses of the system under various constitutive regimes or loads. This talk will introduce the recently-released 3D version of this tool, with an emphasis on the built-in thermal and mechanical capabilities, as well as a description of the application interface which allows the software to be extended by users.

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

Title: On the Geometry of Dissipative Evolution Equations

Author(s): Celia Reina, *U. Pennsylvania*; Johannes Zimmer, *U. Bath*.

The modeling of continuum dissipative evolution equations remains a challenge and is currently based on phenomenological constitutive relations such as Fourier's law for heat transfer. In this talk we present some connections between the geometry of dissipative gradient flows, the principle of maximum entropy production, large deviation principles for stochastically augmented evolution equations and fluctuation-dissipation relations.

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Title: Mechanical Investigation of Bouligand Microstructures

Author(s): Nobphadon Suksangpanya, Nicolas Guarin, Michael Jones, Pablo Zavattieri, David Restrepo, *Purdue U.*; Nicholas Yaraghi, David Kisailus, *UC Riverside*.

The stomatopods are a group of highly aggressive marine crustaceans that use their 5-mm wide light-weight appendages, made of an ultra strong organic-inorganic bouligand structure, as a hammer to smash their heavily shelled preys with accelerations of a .22-caliber bullet producing forces of 0.5 to 1.0 kilonewtons. This hammer, so called dactyl club, is capable of enduring the incredibly high speeds with tremendous forces from its smashing blows creating excessively high internal stresses without inducing damage. Thus, understanding the structure-property relationships in these extremely strong biological structures may provide critical insight into the development of the high-performance and multifunctional biomimetic materials. This talk will focus on the numerical modeling and mechanical analysis of these Bouligand structures under impact condition to understand the fracture and wave propagation behavior. We successfully combined computational and analytical modeling, 3D printing and mechanical testing to evaluate some important hypotheses about the key morphological features of the microstructure and most important toughening mechanisms that are unique in these hierarchical materials.

Title: 'From Discrete Models with Rotational Degrees of Freedom to Cosserat Continuum through Mathematical Homogenization'

Author(s): Roozbeh Rezakhani, Gianluca Cusatis, *Northwestern U.*

Most of the natural and industrial materials are heterogeneous at a certain scale, and some of their specific macroscopic behaviors during damage are strongly influenced by their micro structural behavior. In this research, multiscale mathematical homogenization technique is used to homogenize fine-scale discrete models, such as the Lattice Discrete Particle Model (LDPM), that has been successfully formulated to simulate concrete and other quasi-brittle materials at the scale of the major heterogeneities. The Lattice Discrete Particle Model (LDPM) simulates concrete at the meso-scale considered to be the length scale of coarse aggregate pieces. In discrete models like LDPM, the displacement and rotation fields are only defined at a finite number of points representing the center of coarse aggregate particles. The homogenization theory has been used to build a multiscale framework to model heterogeneous materials at different scales. The basic idea of homogenization is representing each integration point in the macroscopic domain by a representative volume element (RVE). The RVE is a volume of the material in which related heterogeneity is modeled, while the material is assumed to be homogeneous at the corresponding macroscale point. Deformation gradient at integration points of the macroscopic domain is the input for the solution of the fine-scale problem formulated at the RVE level. Next, using an averaging scheme, the macroscopic response derived from RVE is transferred back to the macro-scale. In this research, a homogenization scheme based on the asymptotic expansion of displacement and rotation fields is developed for discrete models through the classical mathematical homogenization. LDPM is homogenized into a Cosserat continuum in which rotational degrees of freedom exists in addition to the translational ones. In each computational step, macroscopic strain and curvature tensors are applied on the RVE, and the homogenized stress and moment stress tensors are calculated based on the formulations derived in the theory. Fine-scale and multiscale simulations of typical laboratory tests are performed to validate the developed scheme. In addition, elastic and nonlinear properties of homogenized Cosserat continuum is investigated through coupling of material RVE to a macroscopic Cosserat tetrahedral element.

Title: New Stabilized Level-Set Formulation for the Simulation of Newton and Non-Newtonian Fluids and Multi-Materials

Author(s): Stephanie Riber, Rudy Valette, Elie Hachem, *Mines Paristech*.

The analysis of multi-materials flows has attracted considerable attention during the past few decades, particularly in view of industrial and environmental applications such as the behaviour of heterogeneous granular solids and powders, material coating and many others. Indeed, the presence of sharp interfaces and discontinuities are known to be challenging to simulate and thus different approaches are still investigated. In this work, we propose to study and to simulate such multi-materials flows. Therefore, we propose first a robust interface tracking method needed to follow efficiently and accurately the interfaces, but also to consider carefully high jump of different materials properties (different law behavior). It is based on the use of a new modified convection-reaction equation that enables a direct localized levelset re-initialization. Then, we propose an anisotropic a posteriori error estimator that controls the errors at the interface and in highly physical areas. Finally, the stabilized finite element method to solve the transport equation and the Variational Multiscale method to solve the Navier-Stokes equations are adjusted to account for these modifications and to support highly stretched elements with an anisotropic ratio of the order of $O(1 : 1000)$. These improvements have been validated on granular flows from dry state to semi-liquid state, which turns into a Bingham yield stress model. Moreover, we will extend the formulation to simulate complex fluids flow on another Newtonian fluid subject to atmospheric pressure, with the use of two Level-Set functions. Simulations show good results on volume and mass conservations, which validate the method robustness.

Title: Dynamic Finite-Element Analysis of the Axial Resistance of Steel Sheet Pile Foundations Under Impulse Loads

Author(s): Corey Rice, Matthew Whelan, Ph.D., Miguel Pando, Ph.D., Vincent Ogunro, Ph.D., *UNCC*.

Within the U.S., typical foundations of bridge abutments consist of H-piles, typically driven by impact or vibratory installers, to carry the vertical bearing loads of the bridge. Additionally, Z-section steel sheet piling abutment facing is routinely used for scour control in short span bridges, but consideration of the additional contribution to the bearing capacity offered by sheet piles is usually not included in the design calculations. However, several European countries have used steel sheet piles as the sole bearing element of bridge abutments and, recently, several projects within the U.S. have also explored this innovative foundation design. One reason for the limited use of sheet piles as a primary bearing foundation system within the U.S. is the lack of reliable analytical and design procedures validated by experimental test programs. Furthermore, guidance on field estimation of the axial capacity of installed sheet piles from dynamic test data is limited and crucial to ensuring that economical designs can be developed with using sheet piles as the primary bearing elements. This presentation will provide an overview of experimental and analytical research on the behavior of steel sheet piles in cohesionless soil under the action of impulse loads, typical of pile driving and dynamic testing. The fundamental basic research objective is to accurately assess the axial capacity of such piles contributed by end bearing and side friction, while the applied research objective is to produce guidance on the interpretation of dynamic test data for rapid experimental assessment of driven pile capacities. A LS-Dyna finite element model of this system, consisting of a sheet pile wall in a well-characterized soil medium, with essential and appropriate contact algorithms, will be presented and the dynamic damping and mass effects of the soil-structure interaction problem will be analyzed and discussed. The results from this study will allow for the development of dynamic properties, which can be used in the design and field evaluation processes. From this model, appropriate conclusions can be made regarding the suitability of applying extensions of current analysis, design, and field testing techniques used for bearing piles to sheet pile elements. Key words: Sheet Piles, Sheet Pile Abutments, Sheet Pile Axial Resistance, LS-Dyna, finite element modeling, soil-structure interaction, dynamic soil-structure interaction

Title: Inexact Full-Space Methods for Simulation-Based Inverse Problems and Large-Scale Optimization

Author(s): Denis Ridzal, *Sandia Nat'l. Lab.*

The formulation of design, control and inverse problems as constrained optimization problems involves dependent variables, also known as the state variables, and independent variables, such as the design and control variables or model parameters. It is common in practice to eliminate dependent variables from the formulation, through a nonlinear solution procedure, thus replacing the original optimization problem with one that is posed in terms of independent variables only. In contrast, full-space methods treat the optimization problem in its original form, i.e., they simultaneously adjust dependent and independent variables at each iteration. In addition to avoiding expensive nonlinear solves, full-space methods gain full control of the accuracy of linear system solves performed in the course of optimization. Inexact full-space methods aim to exploit inexactness in the iterative solution of linear systems, thereby enabling efficient and robust simulation-based optimization at the large scale. We discuss a hierarchy of inexact full-space methods known as inexact sequential quadratic programming (SQP) methods, and review recent algorithmic and theoretical advances. The hierarchy is based on the increasing complexity of linear systems, and, likewise, the increasing flexibility in the design of efficient solvers and preconditioners for large-scale optimization. We examine the performance of inexact SQP methods on a variety of inverse and design problems based on partial differential equation (PDE) models, with particular emphasis on nonlinear PDE models. We also discuss the implementation of full-space formulations and methods in Sandia's Rapid Optimization Library (ROL, Trilinos), enabled through the SimOpt interface for simulation-based optimization.

Title: A Multi-Scale Model for the Thermomechanical Response of Materials

Author(s): Julian J. Rimoli, Jean-Baptiste Bouquet, *Georgia Inst. Tech.*

We present a length-dependent model for the thermomechanical response of materials through a concurrent multiscale scheme that accounts for: (i) the locally varying values of the sub-grain thermal conductivity tensor due to the interaction of phonons with microstructural features such as grain boundaries, and (ii) a continuum model of thermal stresses that explicitly resolves the polycrystalline structure of the material. At the sub-grain level, we compute the values of the thermal conductivity tensor using the Boltzmann transport equation under the relaxation time approximation. At the continuum level, the polycrystalline structure of the specimen is resolved explicitly by a finite element mesh and the texture of the polycrystal is assumed to be given. At this level, we adopt a Fourier model of heat conduction which utilizes values of thermal conductivity obtained at the lower scale. The mechanical response of the grains is modeled as elastic and anisotropic. The capabilities of the model are demonstrated through a series of examples, which highlight the potential of our approach for designing materials with improved thermomechanical response.

Title: Topology Optimization to Enable Qualification of Additively Manufactured Components

Author(s): Joshua Robbins, Thomas Voth, *Sandia Nat'l. Lab.*

Additive Manufacturing (AM) expands the engineering design space by enabling creation of freeform geometries that can be driven by performance requirements rather than manufacturing constraints. Widespread adoption of this technology has been slow due to limitations in printed material quality and accompanying difficulties in part qualification. The most common approach in overcoming this qualification challenge is to pursue improvements in AM processes and resulting material quality. Alternatively, material imperfections (porosity, inclusions, texture, etc.) can be incorporated into the design optimization problem so that designs are robust to deviations from the ideal material, thereby enabling the use of AM technology "as-is". We will present recent work in the development of optimization based design tools that facilitate component qualification by accounting for AM material quality in the optimization process. By composing objectives that reflect details of the as-printed material, designs can be computed that i) use existing, well characterized AM processes, and ii) meet essential performance requirements. A hierarchical approach is used to design parts based on homogenized parameters that are determined from direct simulations of material microstructure. Peak fields are then computed not from the homogenized simulation but from predicted micro-scale quantities. Example applications will be presented to demonstrate the approach. 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: Drop Circulation in Hele Shaw Flow

Author(s): Scott Roberts, Christine Roberts, Rekha Rao, *Sandia Nat'l. Lab.*

Microfluidic devices are high shear, controlled environments that are useful for studying interfacial mass transport. Two-phase flow of droplets in a rectangular channel is simulated using a stabilized arbitrary Lagrangian-Eulerian (ALE) finite element method, allowing investigation of the 3-D droplet flow patterns. A unique controller is used to enable ALE simulation of a moving drop without the need for remeshing. These simulations are compared to particle-tracking experiments, allowing the identification of multiple internal flow regimes. This research is supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. 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.

Title: A Residual Based Variational Multi-Scale Method Formulation for Nondilute Polydisperse Turbidity Currents

Author(s): Soulemayne Zio, José Camata, Gabriel Guerra, Henrique Costa, Renato Elias, Fernando Rochinha, Alvaro Coutinho, *U. Federal-Rio de Janeiro.*

Sediment transport by turbidity currents are of great importance in the formation of the coastal morphology, and their understanding might contribute significantly to the localization of areas prone to host hydrocarbon reservoirs. The turbidity currents are modeled here in a Eulerian framework by the coupling of Navier-Stokes equation with advection-diffusion equations that describe the polydisperse mixture representing multiple grain size sediment transport. In this work, we extend our Residual-Based Variational Multiscale Formulation (RB-VMS) for the accurate prediction of sediments transport to situations in which the mixture of water and sediments is denser, like what typically happens near the sea bottom. Locally, the particle-particle interaction can no longer be ignored, and different aspects like the increasing of the effective viscosity have to be taken into account. A phenomenological law for the viscosity depending on the sediment concentration is employed, giving rise to a new term of interaction between fluid and sediments. Particular attention is devoted to the subgrid modeling that naturally emerges from the multiscale splitting and to the interaction between turbulent structures and deposition patterns. Near the bottom, this interaction leads to stratification of the flow and loss of the turbulent intensity.

Title: Cellular Materials that Exhibit Phase Transformations

Author(s): David Restrepo, Pablo Zavattieri, *Purdue U.*; Sara Rodriguez, Juan Gomez, *U. EAFIT*; Niles Mankame, *General Motors*.

Active materials like shape memory, ferroelectric and magnetostrictive alloys obtain their characteristic properties due to phase transformations. In these materials, phase transformations occur by changing the packing arrangement of the atoms in a process that resembles multistable mechanisms switching between stable configurations. A similar behavior has been observed in folded proteins in which phase transformations (i.e. the change from folded to unfolded configuration) provide the mechanisms through which biological materials obtain remarkable properties such as combinations of strength and toughness, superelasticity and shock energy dissipation, among others. We extend the notion of phase transformations to periodic cellular materials by introducing materials whose unit cells have multiple stable configurations. Each stable configuration of the unit cell corresponds to a phase, and transitions between these phases are interpreted as phase transformations for the material. In this work, we present a cellular material that exhibits phase transformation and use computational simulations and analytical models to understand the underlying mechanics of the unit cell that allows the material to present phase transformations. Also, using computational models we studied the quasi-static behavior of this material and analyzed its wave propagation characteristics using Bloch- periodicity analyses implemented in a finite element framework. Preliminary results show that this material is characterized by a long serrated loading and unloading plateaus, exhibit hysteresis under cycling load and the phase transformation alters the preferential direction of wave propagation at certain frequencies. An attractive feature of these materials is that these behaviors are obtained without inelastic deformation of the base material.

Title: Comparison in 3D of Microstructural Evolution in Deformation with Simulation

Author(s): Anthony Rollett, Robert Suter, *Carnegie Mellon U.*; Reemu Pokharel, Ricardo Lebensohn, *Los Alamos Nat'l. Lab.*

We will summarize the current state of comparisons between experiments and simulations of deformation of polycrystalline materials and provide a more detailed account of an experiment with a tensile test on copper. Polycrystal plasticity is akin to deformation of a composite in which each grain has different properties by virtue of its anisotropic response to loading. It is important to demonstrate that we can validate crystal plasticity simulations in order to relate damage initiation such as cracks and voids to extreme values in stress, for example, as they relate to microstructural features such as triple lines. The specific example is for a tensile test on a pure copper sample that used High Energy Diffraction Microscopy (HEDM). For the simulations, the mechanical response used a spectral method based on Fast Fourier transforms (FFT), which uses the measured image of the undeformed material directly. Various measures of heterogeneity such as maps of grain average strain, kernel average misorientation (KAM), grain orientation spread (GOS), intragranular grain misorientation (IGM) can be used to make comparisons. These measures involve differentiation of the orientation map, which tends to amplify the noise in the maps. Comparing the magnitude of the lattice rotation on a pointwise basis, however, gives more useful results and integrates, in effect, the effect of the accumulated slip over the strain interval considered. Variations in the simulations include strain gradient, stress gradient, isotropic hardening, latent hardening as constitutive models, and viscoplastic versus elasto-viscoplastic methods. The comparisons between experiment and simulation will be evaluated. In general, it is already known that crystal plasticity simulations give good results at the statistical level (e.g. texture development) but indifferent agreement at the local (grain) scale. Also, both experiments and simulations show that hot spots in stress or elastic energy density occur close to grain boundaries, triple lines and quadruple points. Although correlations are found between hot spots and interfaces, special boundaries do not appear to play any role. Support from AFOSR, DOE/BES, NSF, NDSEG and LANL is gratefully acknowledged. Discussions with, and help from Chris Hefferan, Jon Lind, Ulrich Lienert, Frankie Li and many others are gratefully acknowledged.

Title: Application of the Direct Flux Reconstruction Method to the Euler Equations

Author(s): Joshua Romero, Antony Jameson, *Stanford U.*

In recent years, the flux reconstruction (FR) methodology [1] has proved to be an attractive approach for obtaining high-order solutions to hyperbolic partial differential equations. One of the barriers to the more widespread utilization of this method and other high-order methods is their complexity in implementation relative to existing low-order schemes. Recently, a modified approach to FR has been developed, referred to here as the direct flux reconstruction (DFR) method, which simplifies the implementation by replacing the application of correction functions in the standard FR approach with a single Lagrange interpolation operation. This modified scheme has been proven to recover the FR formulation of the nodal discontinuous Galerkin (DG) scheme and also proven to maintain linear stability properties in this case. Additionally, a new family of linearly stable schemes enabled through this methodology has been identified through von Neumann analysis for one-dimensional linear advection problems with particular variants of this method exhibiting super convergence rates greater than the DG method for these problems. Previous work on this scheme thus far has been limited to one-dimensional analysis. The current work will focus on applying the DFR method on quadrilateral grids using a tensor product formulation to the Euler equations. A brief overview of the DFR procedure, with respect to the standard FR approach will be described, as well as the extension to quadrilateral elements using tensor products. Following this, an investigation into the performance of this scheme for solving the Euler equations will be described. Numerical experiments using an isentropic vortex test case on a Cartesian grid [2] will be carried out to characterize the order of accuracy of the formulation, with comparisons drawn between several variants of the DFR method. Additional discussion will follow comparing the order of accuracy results obtained in two-dimensions to those obtained for linear advection in one-dimension. Furthermore, the results of applying this method to the computation of inviscid flow around a circular cylinder will be presented to further demonstrate the performance of the DFR method in this setting. References: 1. Huynh, H.T.: A Flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods, AIAA Conference Paper, 2007-4079 (2007) 2. Vincent, P.E., Castonguay, P., Jameson, A.: Insights from von Neumann Analysis of High-Order Flux Reconstruction, J. Comput. Phys., 230, 81348154 (2011)

Title: Thermodynamically Consistent Integrators for Non-Smooth Coupled Problems

Author(s): Ignacio Romero, Elena Pastuschuk, Juan Carlos García Orden, *Technical U. Madrid.*

Energy and momentum conserving algorithms have been quite successful within the Computational Mechanics and Multibody Systems communities. Not only they are capable of exactly preserving the conservation laws of momenta and energy, but exhibit a remarkable numerical robustness that makes them ideally suited for stiff problems in dynamics. In [1] we extended these methods to coupled problems in thermomechanics, leading to so-called Energy-Entropy-Momentum (EEM) methods that, for closed systems, provide numerical approximations that in addition to preserve momenta and energy, guarantee unconditional satisfaction of the second law of thermodynamics. Like their conserving counterparts, the thermodynamically consistent method show a stable behavior for time steps which are often much larger than what's affordable for standard implicit methods. Energy-Entropy-Momentum methods have been developed for smooth thermomechanical [2] and phase field problems [3]. In the current work, we present an extension of these algorithms to a non-smooth case, the elasto-plastic problem, developing the general theory and illustrating its performance with a model example. We explain how, by a correct generalization of the formulation using non-smooth calculus, the same ideas leading to known EEM methods can be generalized. The result is a very general strategy for developing structure preserving methods that can be applied to most problems of interest in mechanics. [1] Romero, I. (2009). Thermodynamically consistent time stepping algorithms for nonlinear thermomechanical systems. *International Journal for Numerical Methods in Engineering*, 79(6), 706–732. doi:10.1002/nme.2588 [2] García Orden, J. C., & Romero, I. (2012). Energy-Entropy-Momentum integration of discrete thermo-visco-elastic dynamics. *European Journal of Mechanics - a/Solids*, 32, 76–87. [3] González-Ferreiro, B., Gomez, H., & Romero, I. (2014). A thermodynamically consistent numerical method for a phase field model of solidification. *Communications in Nonlinear Science and Numerical Simulation*, 19(20), 2309–2323.

Title: Mechanical Properties of Organic Electronic Materials: A Coarse-Grained Molecular Dynamics Study

Author(s): Samuel Root, Darren Lipomi, Gaurav Arya, *UC San Diego*.

Interest in organic electronics stems from the potential to use solution-processable organic materials to manufacture mechanically compliant thin-film electronic devices. To realize this potential it is necessary to design new organic semiconductors and composites that are mechanically robust enough to withstand the strains associated with processing, along with those of portable and outdoor applications. In this study, coarse-grained molecular dynamics (CGMD) simulations are used to investigate the mechanical properties of organic photovoltaic bulk heterojunctions. Using P3HT: PCBM as a model system, the predictive capabilities of non-equilibrium CGMD uniaxial strain deformation simulations are evaluated through comparison to experimental data. The calculated tensile modulus is shown to be in good agreement with values measured experimentally using the mechanical buckling method. In addition to this, important mechanical properties—unattainable from thin film mechanical experiments—such as yield point, ultimate strength, and degree of chain alignment due to strain-induced plastic deformation are calculated. The framework developed in this study points toward a new design methodology for organic electronic material systems, where bulk mechanical and electronic properties for potential new molecular structures can be predicted a priori in order to facilitate the design of “molecularly stretchable” semiconducting materials. These simulations can easily be extended for modeling small molecule, all-polymer, and block-copolymer systems.

Title: Non-Linear Probabilistic Analysis of Concrete Wall Structure Safety Under Aircraft Impact

Author(s): Peter Rosko, *Vienna U. Tech.*; Juraj Kralik, *Slovak Tech'l. U.-Bratislava*.

The contribution presents the nonlinear probabilistic analysis of the reinforced concrete wall structures under aircraft impact. The dynamic load is defined in time domain on the base of the airplane impact simulation considering real stiffness, mass, direction and velocity of the flight. The dynamic response is analyzed in the system ANSYS using the transient nonlinear analysis solution method. The damage of the concrete wall is evaluated in accordance with the standard NDRC considering the spalling, scabbing and perforation effects. The calculation of the probability of structural failure under extreme loads is based on the probabilistic safety assessment (PSA) level 2. The inaccuracy of the structural model and resistance are determined by the quality of the analyzed model and numerical methods. The uncertainties of the loads level (airplanes velocity and flight direction, dead and live loads), the material model (concrete cracking and crushing, properties 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 coefficients 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 simple and detailed analyses of the wall damage are compared.

Title: A Simple Linear Tetrahedral Finite Element Method for Non-Linear Implicit Elastodynamics

Author(s): Simone Rossi, Nabil Abboud, Guglielmo Scovazzi, *Duke U.*

We present a new tetrahedral finite element formulation for implicit nonlinear hyper-elasticity using piecewise linear continuous shape functions. In order to enhance the performance of low-order tetrahedral elements for nearly-incompressible and incompressible motion, we employ a mixed velocity/pressure formulation. For isotropic hyperelastic materials, the spherical component of the stress is directly associated with changes in volume, and therefore the pressure is strictly associated with the volumetric part of the strain-energy function. Under dynamic conditions, the volumetric energy also defines a rate equation for the pressure which is tightly coupled with the momentum equation. The fully implicit P1/P1 approximation of the velocity/pressure-rate formulation is not LBB stable, and, to overcome this problem, we use a variational multiscale stabilization method based on a consistent linearization of the pressure equation. We show several numerical experiments to demonstrate the performance of the proposed method under dynamic and quasi-static conditions using different volumetric constitutive models. For its simplicity, the proposed method is well suited for dealing with large scale problems on complex geometries.

Title: Three-Dimensional Concrete Crack Propagation Using Transition from Continuous Damage to XFEM

Author(s): Simon-Nicolas Roth, *Hydro-Québec*; Azzeddine Soulaïmani, *ETS Mtl.*; Pierre Léger, *E. Polymtl.*

This work presents the development of a three dimensional concrete cracking simulation strategy based on a transition from continuum damage mechanics to cohesive XFEM approach. The continuous damage model (CDM) provides a relatively good model to describe, in the idealized fracture process zone (FPZ), the formation and growth of densely distributed microcracks. However, in the final stage of failure, when damage localizes into a macroscopic crack, the continuum models are known to exhibit stress locking (spurious stress transfer), lack of objectivity (mesh-induced directional bias), and possible instability (appearance of spurious kinematic modes). Using energy conservation enforced for mode I energy dissipation, the proposed model uses a transition to a cohesive XFEM approach to model the macroscopic crack. The proposed model combining CDM with XFEM in one single approach provides a good technique to describe the complete failure process of quasi-brittle materials. This approach was successfully applied in two-dimensional space [1] and is extended in three dimensional space in this work. Compared to 2D applications, the complexity to track the crack path in 3D presents a great challenge to solve. The use of a global tracking algorithm, helps define a continuous and unique smooth, planar or curved crack surface at the cost of having to solve an additional global system of equations. The global tracking algorithm solves a heat conduction like problem to provide a scalar level set function computed on the basis of the conductivity matrix defined by the principal stress directions. After this additional problem is solved, the 3D crack path is defined from the isosurface extending the crack surface using a marching cube algorithm [2]. Using the proposed combined XFEM-CDM approach, we would like to share our experience on the numerous challenges that must be overcome to successfully model non planar crack propagation in three dimensional space. Numerous three dimensional test cases with non-planar crack surfaces are presented to perform verification and validation of the proposed model. [1] S-N. Roth, P. Léger, A. Soulaïmani (2015), A combined XFEM-damage mechanics approach for concrete crack propagation, *Computer Methods in Applied Mechanics and Engineering*, 283: 923-955 [2] C. Linder, and X. Zhang (2013), A marching cubes based failure surface propagation concept for three-dimensional finite elements with non-planar embedded strong discontinuities of higher-order kinematics. *Int. J. Numer. Meth. Engng.*, 96: 339-372

Title: Modeling Projectile Penetration Mechanics in a Mesh-Free Computational Framework

Author(s): Michael Roth, Jesse Sherburn, Thomas Slawson, *US Army ERDC*; J. S. Chen, Michael Hillman, *UC San Diego*.

Material and structure response to extreme events like explosive detonation and projectile penetration is an area of significant interest to the engineering and scientific communities. The analysis of system response necessitates robust methods to accurately model the complex phenomena that dominate these extreme events. For projectile penetration and perforation, the target and penetrator failure mechanisms, coupled with the material response to high-rate impact loading, are crucial parts of the penetration mechanics. The ability to accurately model this complex behavior: 1) is critical for reliable analysis and design, and 2) presents unique challenges for the development of accurate and robust numerical techniques. The actively developing class of meshfree methods provides new capabilities in this field by naturally capturing large deformation and material separation without nonphysical treatments required by other approaches. To advance computational capabilities for high-rate penetration modeling, a new Reproducing Kernel Particle Method [1] impact and penetration formulation [2] has been developed. A stabilized semi-Lagrangian formulation is utilized for accurate numerical integration in the presence of material fragmentation, and evolutionary contact conditions between target and penetrator are addressed through a contact algorithm that obviates the need for a priori contact surface definitions. Penetration into concrete is of specific interest, so a multiscale material damage model [3] that links continuum-scale damage with microstructure fracture is also implemented. Projectile impact experiments into materials with differing strength and ductility are simulated for comparison of energy attenuation and failure modes as a function of the penetration event parameters (geometry, velocity, and target material properties). Results cumulatively validate the formulation accuracy for these type of extreme events. Permission to publish was granted by Director, Geotechnical and Structures Laboratory. References [1] J. S. Chen, C. Pan, C. T. Wu and W. K. Liu, Reproducing kernel particle methods for large deformation analysis of nonlinear structures. *Comput. Methods in Appl. Mech. Engrg.*, Vol. 139, pp. 49-74, 1996. [2] P. C. Guan, S. W. Chi, J. S. Chen, T. R. Slawson, and M. J. Roth, Semi-Lagrangian reproducing kernel particle method for fragment-impact problem. *Int. J. Impact Eng.*, Vol. 38, pp. 1033-1047, 2011. [3] X. Ren, J. S. Chen, J. Li, T. R. Slawson, and M. J. Roth, Micro-cracks informed damage model for brittle solids. *Int. J. Solids Struct.*, Vol. 48, pp. 1560-1571, 2011.

Title: Virtual Laboratory Based on a Coupling of DEM and MAC Methods

Author(s): Varvara Roubtsova, Mohamed Chekired, *IREQ*.

The study of soil stability under water flow is a complex problem in geotechnical sciences. Phenomena such as liquefaction, internal and external erosion are the result of interaction of soil particles with water flow. A virtual laboratory has been developed to help understand these processes at micro scale. Codes for the virtual laboratory are based on coupling of two well-known methods: Discrete Element Method (DEM), which simulates particle movement using Newton's laws, and Marker-And-Cell (MAC), which models the transient viscous water flows by solving the Navier-Stokes equations. Particle influence on water flow was taken into account by utilizing special non-slipping conditions. Conversely, the drag force acting on a particle due to water flow was calculated by integrating the pressure field and viscous stresses around a particle. Special algorithms were developed to study real geotechnical problems. For example: two different methods for creating virtual samples of soil with given porosity and particle-size distribution (PSD) were developed for 2D and 3D cases. One is based on a fractal model and the second on the real process of particles falling under gravity. A special technique to trace the streamlines was developed to study the real tortuosity in porous media. Ongoing comparison of results obtained by simulation with theoretical and experimental data was carried out during development of the virtual laboratory. The most interesting results presented include the study of particle interaction with a viscous fluid, testing permeability using tortuosity analysis, and creation of soil samples with differing porosity. The virtual laboratory developed here suggests the feasibility of studying parameters difficult to quantify in real experiments. To illustrate this possibility the full energy balance during normal and tangential interaction of particles is shown. This study was used for an analysis of a work of external forces to a change of internal particle energy during a standard shear stress experiment. The full equilibrium of internal and external forces as well as the force distribution in a shear box and the equilibrium of work of external force vs variation of internal energy is presented. The main technical characteristics of the virtual laboratory, such as high parallel programming using GPU devices and visualization using Alioscopy technology, will be briefly described.

Title: Constrained Topology Optimization Using Multi-Point Perturbations of Global Variables

Author(s): Willem Roux, *LSTC*.

The constrained topology design of highly nonlinear problems – for example, crash – has two complications: the difficulty of computing the design sensitivities and the existence of multiple equilibrium paths. Some of our recent work focused on the constrained topology optimization using the numerical derivatives with respect to global variables such as part mass fractions and load case weights. This approach has two sets of variables, the global variables which are set to satisfy the constraints, and the local variables such as the element density which describes the topology or layout. The global variables are computed using standard mathematical programming together with numerical derivatives and the local variables are computed using any standard topology design algorithm such as fully stressed. This approach is successful for both linear and nonlinear structures alike. However for some highly nonlinear problems, the perturbations of the global variables yields different equilibrium paths, and derivatives computations are not meaningful. In these cases the emphasis shifts to finding a design with the best equilibrium path, and this is done adjusting the global variables in a organized random search. This paper gives the general approach constrained topology optimization using multi-point perturbation of global variables, continues into a specific multi-point version for multiple equilibrium branches, and finally illustrates using a simple linear example problem and a highly nonlinear structure with two collapse mechanisms.

Title: Cavitation Pitting: Using the Target Material as a Sensor

Author(s): Samir Chandra Roy, Marc Fivel, Jean-Pierre Franc, Christian Pellone, Marc Verdier, *U. Grenoble Alpes*.

Cavitation erosion results from complex fluid/structure interaction due to multiple bubble collapses near the surface. Numerical prediction of mass loss due to cavitation erosion requires the knowledge of hydrodynamic impact loads generated by each bubble collapse. A new method is proposed to estimate cavitation impact loads from statistical analysis of the pit geometries (characterized by pit depth and diameter). The method is based on an iterative inverse FEM modeling of the material response to a representative Gaussian pressure field. The pitting tests used in this analysis consist of short duration cavitation erosion tests so that each pit is considered to be the plastic imprint of a single impact. It is found that the Gaussian pressure field is relevant to the load distribution induced by a single bubble collapse since simulated and experimental pit shape resemble each other. Thus, the impact load distribution resulting from the inverse modeling should reflect the flow condition and should be material independent provided the material constitutive behavior is characterized properly. Pitting tests were done on Aluminum alloy (Al-7075), Nickel-Aluminum-Bronze alloy (NAB) and duplex stainless steel (A-2205). The ranking of the pitting rates (number of pits/cm²/sec) is found to be Al-7075>NAB>A-2205. For all three materials, the constitutive equations were first characterized and the impact loads were estimated using the inverse procedure described above. When the material properties are obtained from uniaxial compression or tension test, the ranking of the yield strengths is not consistent with the ranking of the pitting rates. Moreover, the estimated impact loads are material dependent. On the other hand, when the material properties are obtained from nanoindentation experiments, the ranking of the obtained hardening curves is consistent and the measured impact loads are material independent. We saw that Al-7075 T651 behaves differently in uniaxial loading and under nanoindentation. This could be related to the microstructure. The conclusion is that nanoindentation tests are appropriate to characterize the material behavior for cavitation applications. To account for higher strain rate ($\sim 10^6$ s⁻¹) in cavitation pitting, the materials' strain rate sensitivity was measured from compression tests complemented by Split Hopkinson pressure bar tests done at strain rates ranging from 0.001 to ~ 2000 s⁻¹. The strain rate effect is then introduced in the Finite Element Modeling by using a Johnson-Cook plasticity model. Using a simple damage model, we show that multiple impacts could lead to a mass loss behavior in good agreement with the cavitation erosion tests.

Title: Study of Effects of Void Size and Shock Strength on Shock Initiation due to Void Collapse in Heterogeneous Energetic Materials

Author(s): Sidhartha Roy, Oishik Sen, Nirmal Kumar Rai, H. S. Udaykumar, *U. Iowa.*

Heterogeneous energetic materials like HMX under shock loading lead to the formation of local hot-spots due to energy localization. The temperature at the hot-spot being higher than the bulk material, are potential sites for detonation and deflagration and are critical in controlling the ignition in solid explosives. The temperature of the hot-spots in such materials are observed to be sensitive towards void size and shock strength. The local high temperature regions grow and trigger exothermic chemical reactions leading to ignition and formation of detonation waves in the material. In order to gain a deeper understanding of the physics behind shock initiation and ignition due to void collapse, the present work studies the sensitivity of the maximum temperature of a hot-spot in a heterogeneous energetic material to various parameters, such as shock strength, void size, void arrangement, loading configuration. A parametric study on shock initiation in HMX is conducted using a massively parallel Eulerian code, SCIMITAR3D[1, 2]. The chemical reaction and decomposition has been modeled using Henson-Smilowitz multi step mechanism. The study identifies ignition threshold parametric criteria based on critical void diameter, critical shock strength etc. The study concludes with the construction of a metamodel using the Dynamic Kriging Method [3] which can be used as a presentative pop-plot in multiscale simulations.

Title: A Massively Parallel Terascale Matrix-Free Computational Framework for Phase Field Modeling

Author(s): Shiva Rudraraju, *U. Michigan Ann Arbor.*

Phase Field Models have been central to computational modeling of complex morphological evolution in multiphase solids. Under the aegis of DOE's PRedictive Integrated Structural Materials Science (PRISMS) Center at the University of Michigan, a massively parallel phase field framework PRISMS-PF is being developed. PRISMS-PF is a matrix-free finite element code based on the deal.ii library which provides extensive support for various finite element constructs, peta-scale grid generation with adaptivity, scalable data structures and solvers. While the framework is expected to serve as a generic phase field library with coupled mechanics capability, the initial development focuses on modeling of precipitate evolution in binary and ternary alloys, as well as grain growth and recrystallization. Current code modules include matrix-free implementations of coupled Cahn-Hilliard, Allen-Cahn and Mechanics, with example demonstrations of spinodal decomposition, chemo-mechanical boundary value problems, and beta-prime precipitate evolution in magnesium/rare-earth binary alloys. The parallel performance and scaling has been demonstrated on terascale problems with billions of degrees of freedom running on thousands of processors. In this talk, I will present the numerical framework, matrix-free formulation, scaling studies and applications to various problems in material physics.

Title: Going Beyond the Diameter in Predicting Rupture of Aneurysms: Investigating the Influence of Iliac Artery Occlusion on Hemodynamics and Wall Stresses of Abdominal Aortic Aneurysms

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

Rupture of abdominal aortic aneurysms (AAA) can be life threatening, as ruptured aneurysms carry a 65-80% mortality rate. Despite decades of active research in the AAA field, aneurysm diameter still remains the primary criteria for deciding medical intervention. Clinicians typically intervene when the aneurysm diameter is larger than 55mm or if the aneurysm grows more than 10mm/year. Clinical observations have shown that smaller aneurysms (classified safe because of diameter thresholds) also rupture, motivating the need to look beyond the diameter as a rupture predictor. Furthermore, women are four times more likely to have smaller aneurysms rupturing than men; along with active smokers and patients with high blood pressure. This motivates the need for looking beyond simply the diameter of the aneurysm as a rupture predictor. Our research into patients with smaller ruptured AAA (< 55mm) indicates that over a quarter (26.7%) of patients also have occluded common, internal and/or external iliac arteries, herein collectively called aortic outflow occlusion (AOO). This motivated an in-depth investigation into AAA patient-specific mechanical stresses that included computational fluid dynamics (CFD) and finite element analysis (FEA). CFD analysis of AOO/AAA patients revealed large increases of hemodynamic parameters such as pressure drop across the AAA (> 100% increase) and wall shear stresses (> 50% increase) and also showed different blood flow patterns between normal and occluded geometries. FEA analysis of the arterial wall and thrombus using a newly developed linear modeling approach revealed a modest increase in wall stresses (~ 2.5% increase) because of iliac artery occlusion. Taken together, these results indicate that AOO strongly influences the hemodynamic environment in a patient with an AAA, and could explain the increased risk of rupture. While further investigations are underway, results thus far are promising. Our combined CFD+FEA modeling enables calculation of patient-specific conditions that go beyond the AAA diameter and incorporates other physiologically relevant information such as the presence of AOO in assessing the rupture risk of patients with AAA.

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Title: Testing and Comparing the Augmented Block Cimmino Distributed Solver on Some Class of Applications

Author(s): Daniel Ruiz, Mohamed Zenadi, Ronan Guivarch, *U. Toulouse*; Olivier Boiteau, Robin Greffeuille, *EDF*; Iain Duff, *STFC-RAL, CERFACS*.

We consider the use of the Augmented Block Cimmino Distributed method (ABCD-solver), a hybrid linear solver based on block row-projection techniques of the type of the Cimmino or Kaczmarz iterative methods. The method offers a particular feature, that enables to "embed" the actual linear system to solve in a super-space, adding extra meta-variables, and raising a "pseudo direct" solver in the sense that the method will converge in one iteration only. We describe the way this augmentation process is integrated within the Block Cimmino method, and how this can be managed very efficiently in a parallel environment, because this is actually one of the very important characteristics of the potential of such an approach. Of course, this feature is of interest only in the case when the extra cost induced by this augmentation approach compensates the number of iterations of the usual Block Cimmino method (e.g. using ABCD-solver without the activation of this augmentation feature). This is pretty much application dependant, and we shall investigate the benefits of this in the context of some structural mechanics and fluid mechanics applications developed at EDF, the national center for electrical power in France. We will also compare ABCD-solver with some other existing methods in terms of computations and memory costs, and in terms of parallelism and efficiency as well on some high performance computers. The ABCD Solver package (release 1.0) is freely accessible at <http://abcd.enseeiht.fr>, including installation instructions and documentation.

Title: A Variational Approach to Crystalline Interfaces: A New Method for Predicting Morphology and Relaxed Interface Energy

Author(s): Brandon Runnels, Michael Ortiz, *Calif. Inst. Tech.*; Irene Beyerlein, *Los Alamos Nat'l Lab.*

Interfaces in crystalline materials are at the forefront of research in micromechanics and multiscale modeling. In particular, interfaces with complex morphologies have been observed to play a crucial role in many micromechanical phenomena such as grain boundary migration, stability, and twinning. However, the complex and diverse behavior of interfaces is still an active area of research, and it appears that there are no predictive models for the energy and morphology of interfaces with arbitrary character. We introduce a new model for predicting the energy of an interface of arbitrary character between crystalline materials of arbitrary structure. Building on this general interface energy model, we propose a method for predicting the relaxed energy and morphology of interfaces. We formulate a variational principle for interface energy, and show that the interface energy functional is in most cases nonconvex. Because of this, the functional lacks lower semicontinuity and consequently the infimum is not attained in general. Following the usual approach for treating nonconvexity in mechanics, we propose a faceting construction that recovers the convexification of the interface energy functional, making the problem well-posed. We then formulate the model in a computationally convenient manner and introduce an algorithm for computing the relaxed energy and structure with an arbitrary interface energy model. We then discuss our implementation of the convexification method together with the general interface energy model, and provide results for several examples in various face-centered cubic (FCC) grain boundaries. For symmetric tilt boundaries, we conclude that the relaxation construction greatly improves the energy calculation from the unrelaxed model. For asymmetric tilt and symmetric twist boundaries, we find that the convexification gives good results for the energy and morphology of the interfaces.

Title: Feature-Preserving Spatial Density Tuning of a Maximal Random Disk Packing

Author(s): Ahmad Rushdi, *UT Austin*.

A triangulation (mesh) of a set of generally unstructured well-spaced points has good quality triangles (or tetrahedra), with no small or large angles, and slowly varying edge lengths. These meshes are important for use in the finite element method and other numerical methods for solving partial differential equations. One popular way to build a point set (and a mesh) like that is Delaunay refinement (DR), iteratively adding the center of an empty Delaunay circle as a point. The placement of these centers (vertices) is chosen to enforce boundary conformity and to improve the quality of the mesh. We consider a dual alternative to DR that provides greater flexibility in controlling the local mesh density and quality, based on random disk packing. A disk packing is a set of random disks (filled circles) covering some domain, and is said to be conflict-free if no disk contains the center of another, and maximal if there is not room to add another disk into the domain without creating a conflict. For fixed or slowly varying disk radii, the disk centers of a maximal packing are well-spaced. Different disk packings may have widely different numbers of disks, and density. At one extreme, the disks are tightly packed, touching one another, in a hexagonal packing. At the other extreme, disks are also in a hexagonal packing, but spaced far apart, just close enough that there is no room to add a full disk between them. These vary in density by about a factor of three. For densities away from these extremes, there are many variations of random, unstructured packings that can be achieved. We describe an algorithmic framework for changing (tuning) one maximal packing into another by changing its spatial density, to meet a quality criterion or a user-defined density. This is distinguished from changing the sizing function or radius of the disks. One goal of tuning is to control the number of disks and their density (area fraction covered by a disk). For example, in meshing (as well as computer graphics, etc.), using fewer points while maintaining the well-spacedness property may speed up the simulation. Another example is producing a model of a cross section of a fiber material, the circles representing fiber cross sections. For a simulation involving such a model to be accurate, we need a density and randomness that corresponds to the physical material. Improving the quality of a mesh, we also use tuning to remove non-obtuse angles and increase edge-valence. Starting from any maximal random packing such as MPS (maximal Poisson-disk sampling), we may achieve a user-defined density, either more dense or more sparse, almost up to the theoretical limits. Except in the extremes, we retain some randomness properties of the input packing. Given an existing packing, we iteratively relocate, inject (add), or eject (remove) disks, using a set of three successively more aggressive local operations. We change the density of the packing one disk at a time, maintaining the minimum disk separation distance and the maximum domain coverage distance required of any maximal packing. Our algorithm can handle spatially-varying sizing functions successfully, and can be applied to planar domains as well as curved surfaces.

Title: Effects of Cerebral Autoregulation and Collateral Flows on Intracranial Hemodynamics

Author(s): Jaiyoung Ryu, Shawn C. Shadden, *UC Berkeley*; Xiao Hu, *UC San Francisco*.

The brain has inherent ability to maintain adequate cerebral blood flow (CBF) in various physiological and pathological conditions, such as rapid changes of blood or intracranial pressure, and occlusion of arteries. Important features of intracranial hemodynamics include, (1) cerebral autoregulation (CA; metabolic, myogenic, or neurogenic hemodynamic processes), (2) cortical anastomosis that can transfer blood between different regions of brain, (3) communicating arteries that form the Circle of Willis (CoW) to redistribute blood supply among the major cerebral arteries, and (4) multiple arterial blood sources (carotid and vertebral arteries). The functions of these are highly coupled. In this study, we examine the impacts of acute arterial stenosis or vasoconstriction on intracranial hemodynamics focusing on the role of CA and collateral flows. We employ a one-dimensional (1-D) nonlinear cerebral blood flow model. To consider important aspects of cerebral circulation listed above, 1-D vascular network includes a large range of vessels (aorta/carotid/vertebral/subclavian/brachial arteries, and arteries forming the CoW) and the downstream model is coupled with CA, ICP, and cerebrospinal fluid (CSF) models. Our results show that CA can maintain CBF even in challenging situations (60% MCA vessel area reduction), with approximately 30% larger MCA blood flow than impaired CA case. When MCA is totally occluded, distal collateral pathways can provide 10% normal MCA CBF from anterior to middle part of the brain. ICP increases 4mmHg and 2mmHg with right CCA and MCA occlusions, respectively. Additional results and discussions regarding arterial pulse wave propagation and ICP waveforms are also discussed.

Title: Simulation of Fatigue in Bioprosthetic Heart Valve Biomaterials

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

For the foreseeable future, bioprosthetic heart valves (BHV) fabricated from xenograft biomaterials will remain the dominant replacement prosthetic valve design. However, BHV durability remains limited to 10-15 years. In the present work we utilized a meso-scale structural constitutive modeling approach to formulate a novel approach. We start by observing that exogenous cross links (EXLs) induced in native collagenous tissues induce the following effects: 1) Stiffen the transverse modulus of the collagen fibers to induce a substantial increase in bending stiffness. 2) Stiffen the non-fibrous matrix 3) Increase fiber-fiber interaction stiffness 4) Increase fiber-matrix interaction stiffness We will start with the structural modeling approach to formulate a novel approach, utilizing our extensive experience with BHV tissues, to develop a FDM for the time evolving (i.e. over many thousands of cycles, not beat-to-beat) BHV mechanical properties. A major focus was delineation of the differences in bulk mechanical properties due to tissue-level dimensional and structural changes (i.e. due to permanent set effects) and the intrinsic changes in the constituent fibers. Here, the standard structural model has been extensively modified to include appreciate fiber stresses in the still-undulated state, fiber ensemble and fiber-matrix interactions. Following damage theory convention, we utilized a normalized scalar damage metric variable $D(t)$, which ranges from 0 for new (virgin) material to 1 for completely damaged. We initially assume $D(t)$ follows first-order kinetics, which can be changed to higher order kinetics as needed, with similar expressions developed for each model parameter. As a modification from our original formulation, we note that exogenous chemical cross-links present at the collagen molecular level induce a great increase in effective fiber stiffness, as accounted for using an elastica model. From the pre-implant (virgin) tissue, initial values were obtained from the results of existing data Time course changes obtained for $D(t)$ for each parameter was obtained using extensive existing data from our lab. We were able to quantify, separately, the rates of change in effective fiber stiffness from the changes in fiber splay $R(\blacksquare)$ and collagen fiber recruitment $\blacksquare(E_s)$ and their net contributions to tissue level behavior and durability. The model was then implemented utilized in ABAQUS to simulate the permanent set effects previously observed by our lab. We were able to simulate permanent set effects at the organ level (i.e. prosthetic device). This fact was important in of itself, as changes in prosthetic device level will affect leaflet stress distributions. ACKNOWLEDGMENTS: NIH R01 HL108330.

Title: An Efficient Approach for Stochastic Optimization of Electricity Grid Operations

Author(s): Cosmin Safta, Richard Chen, Habib Najm, Ali Pinar, Jean-Paul Watson, *Sandia Nat'l. Lab.*

The properties of many operational and structural elements of power grid models (e.g., grid topology and state, including knowledge of what lines are down, and what generators/loads are online) are typically known with a relatively high degree of certainty. Other parameters, such as future demand and renewable generation output, can exhibit relatively higher degrees of uncertainty. Stochastic grid optimization problems typically handle these uncertainties in the forecast by considering a number of random realizations from a stochastic process model for uncertain generators or loads in transmission power grids. We propose an approach that can more efficiently handle uncertainty quantification in these models by significantly reducing the requisite number of scenarios (model evaluations) necessary in the stochastic optimization, for a given degree of accuracy in estimated moments of interest. In this work we model uncertain quantities as random variables and employ functional analysis to construct associated spectral Polynomial Chaos (PC) representations in terms of standard random variables. We employ a variance-based global sensitivity analysis to detect important model parameters. We also use Karhunen-Loeve expansions to efficiently represent time dependent wind-generated uncertain power as random fields. We further reduce dimensionality by considering only a number of modes that capture most of the variability in the wind power, while exploiting the dependence between uncertain modes for wind sites that are geographically close. With these representations for uncertain inputs, we employ sparse quadrature for forward propagation of this uncertainty, constructing PC representations for the quantities of interest relevant to the optimization of electric grid operations. We demonstrate these methods on the standard 118-bus IEEE power grid model augmented with several wind-powered generators.

Title: Unconditionally Stable Second-Order Time Integration Algorithms for Coupled Mechano-Chemistry

Author(s): Koki Sagiya, Krishnakumar Garikipati, *U. Michigan*; Shiva Rudraraju, *U. Michigan* .

Many multi-component solids undergo phase-transformations that are driven by diffusional redistribution of their different components coupled with a structural change of the crystallographic unit cell. We here consider an important class of such phase-transformations that is modeled by the mechano-chemical spinodal decomposition. The classical spinodal decomposition is characterized by a chemical free energy that has two wells separated by the "spinodal region." The free energy being concave in the spinodal region with respect to the local concentration of a component, solids with initial concentration in this region experience redistribution of their components to form two separate phases. In the mechano-chemical spinodal decomposition this redistribution of the components is accompanied by the crystallographic structural changes; as the local concentration increases, the mechano-chemical free energy undergoes a continuous transition from convex functions to locally concave functions with respect to appropriate measures of strain, the cubic phase losing stability and transforming into one of three stable tetragonal phases. The concavity in the free energy with respect to concentration and strain respectively lead to ill-posed PDEs for transport, characterized by negative diffusivity, and for mechanical equilibrium, characterized by stress softening. Numerical computations with such PDEs show pathological mesh-dependencies of the computed phase regions, which fail to converge with mesh refinement. This ill-posedness is eliminated by extending the free energy to include dependences on concentration gradients and strain gradients. The resulting PDEs are the Cahn-Hilliard equation for transport and Toupin's formulation of gradient elasticity at finite strains, both of which have fourth-order spatial derivatives. Due to these higher-order derivatives we employ the isogeometric analysis for our numerical simulations. This approach was adopted for general boundary value problems in three dimensions for Toupin's theory in (Rudraraju et al., *Comput. Methods Appl. Mech. Engrg.*, 278:705, 2014). Motivated by the work of (Gómez et al., *J. Comput. Phys.*, 230:5310, 2011), in which a class of unconditionally stable second-order time-discretization methods was proposed for the Cahn-Hilliard equation, we in this work develop a time-integration scheme for the coupled system of the Cahn-Hilliard equation and the strain gradient elasticity that is also second-order and unconditionally stable and demonstrate its ability to solve challenging problems by numerical examples. To our knowledge this is the first stable time-integration scheme for mechano-chemical phase-transformation problems.

Title: Scaling Study of Large Eddy Simulations with Dynamic Models

Author(s): Onkar Sahni, Steven Tran, *RPI*.

We investigate scaling efficiency of parallel large eddy simulation (LES) employing different dynamic models. LES is an attractive method for the simulation of turbulent flows since it provides greater fidelity, which is because in LES the relatively large-scale turbulent flow structures are resolved. However, interactions of the resolved flow structures with those at the subgrid scales are modeled. The modeled/unresolved stresses are based on models which involve constant(s) that may vary in space and time depending on the problem of interest. Multiple choices exist for such models and related to them many dynamic procedures exist for dynamically evaluating the associated constant(s). We consider different dynamic models for LES including the dynamic Smagorinsky model and the residual-based variational multiscale (RBVMS) formulation as well as a mixed model based on the combination of the two. For dynamic procedures, we focus on two averaging and two filtering strategies. The two averaging strategies include spatiotemporal averaging over homogenous directions (if applicable) and Lagrangian averaging (see [1]) over pathlines which is applicable for complex turbulent flows with inhomogeneity. We also study two different filtering schemes including 2D and 3D filtering depending on the underlying structure of the mesh (e.g., 2D filtering in the layered portion of an unstructured boundary layer mesh). We will consider applications ranging from turbulent channel flow to flow over an airfoil. Comparisons with DNS and/or experimental data will be made. References: [1] Meneveau, C., et al. "A Lagrangian dynamic subgrid-scale model of turbulence." *Journal of Fluid Mechanics*, 319:353-395, 1996.

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Title: Cohesive Dynamics for Quasibrittle Fracture

Author(s): Robert Lipton, Eyad Said, *Louisiana State U.*

In this talk we introduce a nonlocal large deformation cohesive model for modeling the dynamics of brittle and quasi brittle fracture. In this model a more complete set of physical properties including elastic and softening behavior are assigned to each point in the medium. We work within the peridynamic framework where strains are calculated as difference quotients. A nonlocal cohesive law relating force to strain provides the constitutive relation. The cohesive law between material points is initially linear for sufficiently small strain after which it becomes unstable and softens beyond a critical strain. At each instant of the evolution the body can be split into a process zone exhibiting nonlinear force-strain behavior and a complementary zone exhibiting elastic behavior. We show that the length scale of nonlocal interaction relative to the characteristic length scales of the sample controls the size of the process zone relative to the sample size. This gives rise to the size effect seen in quasi brittle materials. This theoretical result highlights the role of the peridynamic horizon as a modeling parameter for quasi brittle fracture dynamics. The process zone is shown to collapse onto a set of lower dimension in the limit where the length scale of nonlocal interaction vanishes with respect to the size of the domain. In this "brittle fracture limit," the dynamic evolution is seen to have bounded hyper-elastic energy and Griffith surface energy.

Title: Constitutive Modeling of Hydrogels and Nanocomposite Gels for Designing Layered Composite Structures

Author(s): Trisha Sain, Muhammed Imam, *NCAT*.

Use of layered polymer composites as blast resistant materials has constant demand in defense applications. In order to safely resist the high rate of loading such as blast waves, the constituent materials need to have sufficient stiffness and damping capacity simultaneously. Hence to develop novel materials with enhanced mechanical property, materials with structural hierarchy are designed by optimizing the constituent materials and geometry. In the present study, focus has been given on hydrogels and nanocomposite hydrogels as possible constituents in the layered material system. There has been a significant work in progress in the area of synthesizing strong and tough hydrogels by implementing various energy dissipation mechanisms in the polymer structures such as double network hydrogels, nanocomposite hydrogels etc. In order to design layered materials with multifunctionality such as high stiffness and damping a mathematical framework needs to be developed for characterizing the constitutive response of the constituent materials. A physically motivated mathematical model combined with finite element analysis to optimize the geometry of the layered constituent would also fasten manufacturing of such materials for various engineering applications. In the present study, the goal is to develop a constitutive model for predicting the high rate response of nanocomposite hydrogels. The proposed model is developed in finite deformation framework to incorporate large deformation in the soft hydrogels and gel-type materials. In order to predict the viscoelastic response of hydrogels a time dependent nonlinear stress-strain law is proposed. The constitutive model consists of several branches of spring and dashpot combinations to account for the viscoelastic property in terms of multiple characteristic relaxation times. In order to validate the proposed model, experimental stress relaxation data from literature for covalently crosslinked alginate hydrogel was fitted to find the characteristic relaxation times. For finite element simulations, a 2D plane strain representative volume is chosen which included several layers of polymer materials including hydrogel as the softest layer. The idea here is to maximize shear dissipation due to stiffness mismatch between the successive layers. Eventually a set of guidelines will be developed to design layered composites consisting of hydrogels and nanocomposite hydrogels having stiffness and damping well above the Wang and Lake line. The constitutive model will be extended further to capture the stimuli sensitive response of hydrogels.

Title: An Active Contraction Model of Valvular Interstitial Cells

Author(s): Yusuke Sakamoto, Michael Sacks, *UT Austin*.

Valvular interstitial cells (VICs) play a critical role in the maintenance and pathophysiology of heart valve tissues. When activated, VICs exhibit increased levels of cytokines and extracellular matrix (ECM) synthesis and strong contraction through the expression of α -smooth muscle actin (α -SMA) fibers. The objective of this study was to investigate the roles of different subcellular structures on the VIC mechanical responses under different mechanical loading conditions and activation states. We modeled the VIC as a continuum with two main structures: the cell nucleus and cytoplasm, which occupy distinct domains within the VIC. The nucleus was modeled as an incompressible neo-Hookean material while the cytoplasm was modeled as a mixture of two solid phases: the basal cytoskeleton phase and α -SMA stress fiber phase, which exhibit some orientations and active contraction. Using our VIC mechanical model, we simulated two experiments: micropipette aspiration (MA) and atomic force microscopy (AFM) of the aortic VIC (AVIC) and pulmonary VIC (PVIC) that each exhibits different expression levels of the α -SMA. In the MA experiment, VICs are in inactivated states while in AFM experiment, VICs are in activated states. Using the MA experimental data exhibiting different expression levels of α -SMA, we determined the cytoskeleton shear modulus and the stress fiber intrinsic modulus to be 7.31 Pa and 533.55 Pa, respectively. Using the intrinsic modulus and fiber expression levels, we calculated the effective shear modulus of the stress fibers within AVICs and PVICs as 533.18 Pa and 428.76 Pa, respectively. Here, we assumed that the cytoskeleton shear modulus are constant, and the VICs are inactivated. Thus, only the amount of α -SMA within the VICs contribute to the changes in their mechanical properties. From the AFM data, we determined the contraction strength of AVICs and PVICs were 41.98 kPa and 3.94 kPa, respectively; a ~ 10 -fold difference, implying that not only the expression level of the α -SMA fibers but also the contraction level increases from PVICs compared to AVICs. We also determined the nucleus shear modulus to be 10.69 kPa and 8.43 Pa, respectively, with no statistically significant differences ($p=0.54$). Our model explains this gap between these two measurements by attributing their differences to the active contraction strength of the α -SMA fibers. We also showed that the AVICs exhibit stronger contractile activity than PVICs in activated states. To our knowledge, this is the first study to measure the shear modulus of the nucleus within the cell using AFM.

Title: CUDA Supported Dynamic Functional Connectivity Analysis in fMRI Data

Author(s): Devrim Akgun, *Sakarya U.*; Unal Sakoglu, John Esquivel, Mutlu Mete, *Texas A&M U.-Commerce*; Bryon Adinoff, *UT Southwestern Med'l. Center*; Sinan Kockara, *U. Central Arkansas*.

INTRODUCTION: Increasing the clock speed of the processor is not fashionable way to improve computational performance. Recent advances in multi-CPU processors and graphics card based computational technologies makes dynamic utilization of parallel computing techniques possible. Several applications in various domains, such as bioinformatics, computational mechanics, and computation geometry, were implemented to fasten computationally-intensive solutions, where big data problems are inevitable. However, parallelization of the existing algorithms is a design-demanding task as the performance gain would not be noteworthy if the extend of parallelism of the problem is not methodically analyzed. In functional magnetic resonance imaging (fMRI) based neuroimaging studies, dynamic functional connectivity (DFC) analysis is one of the most computationally challenging algorithms to investigate functional interactions among diverse brain regions or networks identified within fMRI scans. DFC-based analyses help researchers identify pairs of brain areas that are activated or deactivated together over a time-course of experiments. Not only can fMRI data from multiple subjects be quite large (on the order of GBs), but also the number of brain networks and number of combinations of interacting brain networks can be very large (100s of combinations of single brain data)[1]. **METHODS:** In this study, we analyzed and implemented parallel DFC algorithms based on the two different approaches: thread- and block-based. The former once was designed to parallelize each of the fMRI time-course data-points at the lowest level and it was implemented in both Open Multi-Processing (OpenMP) and Compute Unified Device Architecture (CUDA) programming environments. Block-based approach, where parallelization involves shorted parts of fMRI time-courses obtained by sliding windows, is developed to better utilize Graphical Processor Unit (GPU) architecture for certain DFC analysis parameters. **RESULTS:** Experimental results showed that the proposed parallel design solutions enabled by the GPUs significantly reduce the computation time for DFC analysis. Multicore implementation using OpenMP on 8-core processor provides up to 7.7x speed-up. GPU implementation using CUDA yields substantial accelerations ranging from 18.5x to 157x speed-up once thread-based and block-based approaches are combined in the analysis. **CONCLUSIONS:** Proposed parallel programming solutions show that multi-core processor and CUDA-supported GPU implementations accelerate the DFC analyses significantly. Developed algorithms make the DFC analyses more practical for multi-subject studies with more dynamic analyses. [1] Ü. Sakoğlu, G. D. Pearson, K. A. Kiehl, Y. M. Wang, A. M. Michael, and V. D. Calhoun, "A method for evaluating dynamic functional network connectivity and task-modulation: application to schizophrenia," *MAGMA*, vol. 23, pp. 351-66.

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Title: Space-Time, Finite-Element Exterior Calculus and Variational Discretizations of Gauge Field Theories

Author(s): Melvin Leok, Joe Salamon, John Moody, *UC San Diego*.

Many gauge field theories can be described using a multisymplectic Lagrangian formulation, where the Lagrangian density involves space-time differential forms. While there has been prior work on finite-element exterior calculus for spatial and tensor product space-time domains, less has been done from the perspective of space-time simplicial complexes. One critical aspect is that the Hodge star is now taken with respect to a pseudo-Riemannian metric, and this is most naturally expressed in space-time adapted coordinates, as opposed to the barycentric coordinates that Whitney forms are typically expressed in terms of. We introduce a novel characterization of Whitney forms and their Hodge dual with respect to a pseudo-Riemannian metric that is independent of the choice of coordinates, and then apply it to a variational discretization of the covariant formulation of Maxwell's equations. Since the Lagrangian density for this is expressed in terms of the exterior derivative of the four-potential, the use of finite-dimensional function spaces that respects the de Rham cohomology results in a discretization that inherits the gauge symmetries of the continuous problem. This yields a variational discretization that exhibits a discrete Noether's theorem.

Title: Dynamic Design Using Topology Optimization of Laminated Piezocomposites Structures (LAPS) with Coupled Electric Circuits for Energy Harvesting Purposes

Author(s): Ruben Andres Salas, Emílio Carlos Nelli Silva, *U. São Paulo*; Junuthula N. Reddy, *Texas A&M U.*

Laminated Piezocomposite Structures (LAPS) are multi-layer structures composed by piezoelectric, metal and composite materials (epoxy matrix with carbon or glass fiber). These structures acquire improved features over conventional piezoelectric materials because their features cannot be reached by its components in isolated form, for example more generated power and less weight. LAPS are used in energy harvesters devices, which are useful for supplying portable and low power devices, being of great interest the improvement of its dynamic characteristics and performance. Energy harvester modeling request the electric circuit coupled with the structure to estimate the power transfer coming from the LAPS. LAPS dynamic design for purposes of energy harvesting can be systematized by using the Topology Optimization Method (TOM), which is a method based on the distribution of material in a fixed design domain with the purpose of optimizing a cost function subjected to constraints intrinsic to the problem. TOM combines the optimization algorithms and the finite element method (FEM). Thus, this work aims to develop a methodology for dynamic design of Laminated Piezocomposite Structures (LAPS) based on TOM taking into account the circuit coupled with the LAPS. In this work, the TOM formulation proposes to determinate simultaneously, the optimal topology of the materials for different layers, the polarization sign of the piezoelectric material and the fiber angle of the composite layer, in order to design a particular vibration mode for a specified resonance frequency maximizing the energy conversion. In addition, it can be found out the optimum equivalent impedance if the circuit components are treated as design variables. The LAPS modeling is performed by solving the governing equations using the linear FEM based on 3-dimensional 8-node isoparametric elements. In the TOM formulation, several material models are used including the Simple Isotropic Material with Penalization (SIMP) for isotropic materials, the PiezoElectric MAterial with Penalization and Polarization (PEMAP-P) to describe polarization in piezoelectric material and a material based on the Bi-value Coding Parameterization (BCP) scheme for taking into account of fiber orientation in composite materials. The objective function combines harmonic, transient and modal FEM analysis terms to deal with generated power maximization and rise time minimization with the purpose of improving the dynamic response. The transient problem is solved with the Generalized- α time integration scheme and Sequential Linear Programming (SLP) is used for solving the non-linear optimization problem. Results are shown in order to illustrate the method.

Title: A Local Phantom Node Approach for Crack Propagation and Fragmentation

Author(s): Jessica Sanders, Mike Puso, LLNL.

This work proposes a framework for the simulation of dynamic fracture and fragmentation of engineering structures. We present an element-local phantom node method for the three-dimensional description of dynamic crack propagation in a finite element model. Unlike standard XFEM, this method is not based on enforcement of a continuous crack path, or a level set description of crack location. Crack initiation and propagation are based on material laws much in the same way as in strong discontinuity, or enhanced strain methods, and determined on an element-by-element basis. The description of the discontinuity is local to an element. Phantom nodes are nonetheless used to facilitate complete kinematic separation of failed elements. Thus, a free surface is propagated in the material at the site of element failure in the same manner as the XFEM. A prototype of an element-local XFEM was put forth in [1], but with a least-squares notion of crack continuity. Non-continuous cracks have also been represented with partition-of-unity element with internal cohesive zones in two dimensions in [2]. The challenges of handling phantom nodes and a free surface in three dimensions without the benefits of continuity at that surface will be addressed. We will also address various challenges in fragmentation modeling, including the need to adapt to multiple failure models and regularizations, the transition from damage to cracking, and the need to track large quantities of fracture surfaces and new topologies. Various test problems will be presented, with comparisons to standard experimental results in brittle fracture. Extensions to ductile tearing will be discussed. [1] Duan et al. Element-local level set method for three-dimensional dynamic crack growth. *International Journal for Numerical Methods in Engineering* 80, 1520-1543, 2009. [2] Remmers et al. The simulation of dynamic crack propagation using the cohesive segments method. *Journal of the Mechanics of Physics and Solids* 56, 70-92, 2008.

Title: On the Homogenization of Fluid-Filled Deformable Porous Media

Author(s): Carl Sandström, *Chalmers U. Tech.*

Porous materials are present in a large number of engineered as well as natural structures. Various type of filters fall into the first category, whereas bio- and geomaterials are natural ones. The microstructure of this type of materials is strongly heterogeneous, consisting of both a solid and a fluid. As the subscale geometry is generally very complex and at a length scale much smaller than that of the macroscopic applications, it is computationally unfeasible to completely resolve the structure with current computer capacity. Instead, macroscopic material models, which are calibrated from experiments, are used. Although computationally efficient, these models are less flexible in representing the intrinsic physical properties. As a viable alternative, computational homogenization may be used, either in a full-fledged multiscale setting or as a tool to calibrate macroscopic models. Computational homogenization of flow through porous materials consisting of a fluid contained within a rigid solid skeleton is currently well understood and numerous scientific papers has been written on the subject. However, computational homogenization of flows through a deformable solid is still a largely unexplored field. In this work, we start from the fully resolved Fluid-Structure Interaction problem in a porous material and proceed by splitting up the domain into a finite number of subdomains, which eventually, becomes the familiar Representative Volume Element (RVE). The RVE, or subscale, problem is formulated as a monolithic Fluid-Structure Interaction problem where, in order to maintain an admissible computational mesh, a fictitious elastic material is introduced in the pore space of the RVE. By choosing the test space for the subsequent weak formulation in a certain way, the fictitious material does not contribute to the overall subscale stress. The resulting macroscale problem is a modified version of the Darcy flow model, which depends on the macroscale pressure, pressure gradient and deformation. Special attention is given to the numerical estimation of the Biot coefficient.

Title: Stress Fields Induced by a Quadratic Displacement Discontinuity in an Elastic Half Plane

Author(s): Amirhossein Molavi Tabrizi, Ernie Pan, Ali Sangghaleh, *U. Akron.*

This research presents the exact closed-form solutions for the stress fields induced by a two-dimensional (2D) non-uniform displacement discontinuity (DD) of finite length in an isotropic elastic half plane. The relative displacement across the DD varies quadratically. We employ the complex potential-function method to first determine the Green's stress fields induced by a concentrated force and then apply Betti's reciprocal theorem to obtain the Green's displacement fields due to concentrated DD. By taking the derivative of the Green's functions and integrating along the DD, we derive the exact closed-form solutions of the stress fields for a quadratic DD. The solutions are applied to analyze the stress fields near a horizontal DD in the half plane with three different profiles: uniform (constant), linear, and quadratic. The same methodology is applied to an inclined normal fault to investigate the effect of different profiles on the maximum shear stress in the half plane as well as on the normal and shear stresses along the fault. Numerical results demonstrate considerable influence of the DD profile on the stress distribution around the discontinuity.

Title: Unified Thermo-Electro-Magneto-Mechanical Framework for Characterization of Multifunctional Materials

Author(s): Sushma Santapuri, *Polytechnic U. Puerto Rico.*

Multifunctional materials with coupled thermal, electrical, magnetic, mechanical, and/or chemical physical effects have applications ranging from design of novel actuators, advanced sensors, self-healing mechanisms, to energy harvesting devices. The ability to tailor these materials with desired properties using analytical models and computational tools is currently a research area of growing interest and has the potential to accelerate the production of novel advanced technologies. Enabling such an inverse design framework would require the development of multiscale, multiphysics, mathematical models that can integrate the material behavior across various scales of operation and describe the interactions of physical effects involved. To this end, in this work, a broad multiphysics modeling architecture is developed, that can be utilized to characterize multifunctional materials with coupled thermal, electrical, magnetic, and/or mechanical effects, while accommodating both reversible and irreversible material behavior. This is accomplished in a two-step process: firstly, the principles of classical thermodynamics are combined with electrodynamics of continuum to develop a comprehensive thermodynamic framework that characterizes materials exhibiting fully coupled Thermo-Electro-Magneto-Mechanical (TEMM) behavior. Subsequently, constitutive equations for materials undergoing TEMM processes are developed for several special cases, that include (i) reversible (near equilibrium), (ii) transport (flow processes), and (iii) dissipative (irreversible, far from equilibrium) material behavior. This thermodynamic framework is utilized to develop constitutive equations for materials exhibiting approximately reversible TEMM response, and subsequently specialized to small deformations and linear response. The dissipation inequality is utilized to characterize transport processes that include thermoelectric, thermomagnetic, and galvanomagnetic effects. The dissipation inequality is further modified to incorporate spin-related effects. Finally, to extend the framework to hysteretic material behavior an order parameter based phase-field modeling approach is used, and the corresponding constitutive equations are developed. The constitutive models are accompanied by multiphysics interaction diagrams that highlight the various subsets of processes that can be characterized using this framework. The development of this unified thermodynamic framework can accelerate inverse design of novel multifunctional materials. By specifying a targeted application and additional design constraints, the optimized set of material properties can be deduced utilizing the broad energy landscape. Also, this unified thermodynamic framework will provide key insights into behavior of advanced materials and their multiphysical interactions.

Title: Generalized Unified Formulation Shell Element for Functionally Graded Variable-Stiffness Composite Laminates and Aeroelastic Applications

Author(s): Luciano Demasi, *San Diego State U.*; Yonas Ashenafi, *San Diego State U.*; UTC Aerospace Sys.; Rauno Cavallaro, Enrico Santarpia, *San Diego State U.*; UC San Diego.

Composite materials have been extensively used in engineering thanks to their lightweight, superior mechanical performances and possibility to tailor the structural behavior, increasing the available design space. Variable Angle Tow (VAT) structures exploits this advantage by adopting a curvilinear patterns for the fibers constituting the lamina. This work, for the first time, extends the Generalized Unified Formulation (GUF) to the case of fourth-order triangular shell elements and VAT composites. Functionally graded material properties in both the thickness and in-plane directions are also possible. The finite element has been formulated with layers of variable thickness with respect to the in-plane coordinates. GUF is a very versatile tool for the analysis of Variable Stiffness Composite Laminates (VSCLs): it is possible to select generic element coordinate systems and define different types of axiomatic descriptions (Equivalent Single Layer, Layer Wise, and Zig-Zag enhanced formulations) and orders of the thickness expansions. Each displacement is independently treated from the others. All the infinite number of theories that can be generated with GUF are obtained by expanding six theory-invariant kernels (formally identical for all the elements), allowing a very general implementation. Finally, the possibility of tailoring the theory/order to increase the accuracy in desired directions makes the GUF VAT capability a very powerful tool for the design of aerospace structures.

Title: Survey of Numerical Methods for the Stability Analysis Eigenvalue Problem: The 2D Flat Plate Boundary Layer

Author(s): Silvia Sanvido, Eusebio Valero Sanchez, Javier de Vicente Buendia, *UPM*.

Flow stability analysis aims to study the onset of perturbations from a steady state configuration. Small perturbations evolution depends on several parameters: those related to the nature of the flow (Reynolds number, Mach number, etc) and those that describe the geometry (cavity depth, AoA, steps, etc). Linear stability analysis, the temporal approach (Theofilis 2011), defines the flow variables in the equations of motion as a sum of a steady base state and a small amplitude perturbation. When this decomposition is fed into the Navier-Stokes equations it results in a generalized eigenvalue problem (EVP). The imaginary part of the complex eigenvalue from the EVP represents the frequency while the real part is responsible for the growth rate of the, initially small, disturbance. This technique has been successfully applied to simple geometries at relatively low Reynolds numbers. For problems with low degrees of freedom, the EVP can be easily solved either by direct (QZ) or iterative (Arnoldi) algorithms. However, a direct factorization of the matrix is required, making these methods inefficient and even intractable for large 3D problems. The subject matter of this presentation is concerned with devising flexible and accurate numerical methods for the solution of EVP which govern the linear instability of steady flows over complex geometries. Different methodologies for EVP: Shift-and invert, Cayley transform, Jacobi-Davidson approach and several Krylov methods have been studied and confronted (Saad 2003). The benchmark problem examined is the two-dimensional boundary layer flow along a flat plate. Several studies have been performed in the past using this configuration (Ehrenstein and Gallaire 2005). The capabilities of different algorithms have been exploited by increasing the mesh discretisation and consequently the leading dimension of the matrix for the EVP, in order to reach a converged spectrum. Boundary conditions for "open flows" regions have been revisited as they have been proven to have a drastic effect on the eigenspectrum. Two-dimensional results are also compared with those obtained from local analysis (Orr-Sommerfeld equation) and finally, preliminary results for the transient growth from the disturbances recovered in the EVP are presented. Bibliography 1. Global linear instability. V. Theofilis. Annual Review of Fluid Mechanics (2011). Vol 43 pp 319-352. 2. On two-dimensional temporal modes in spatially evolving open flows: the flat-plate boundary layer. U. Ehrenstein and F. Gallaire. J. Fluid Mechanics (2005). Vol 536. pp 209-218. 3. Iterative Methods for Sparse Linear Systems. Y. Saad – 2nd ed(2003)

Title: Density Estimation Framework for Model Error Assessment

Author(s): Khachik Sargsyan, *Sandia Nat'l. Lab.*

In this work we highlight the importance of model error assessment in physical model calibration studies. Conventional calibration methods often assume the model is perfect and account for data noise only. Consequently, the estimated parameters typically have biased values that implicitly compensate for model deficiencies. Moreover, improving the amount and the quality of data may not improve the parameter estimates since the model discrepancy is not taken into account. In state-of-the-art methods model discrepancy is explicitly accounted for by enhancing the physical model with a synthetic statistical additive term, which allows appropriate parameter estimates. However, these statistical additive terms do not increase the predictive capability of the model in general because they are tuned for particular output observables. Further, the arbitrary use of standard additive statistical model error terms on model observables may well violate physical constraints, unless particular care is taken to build in requisite statistical structure to avoid this. In order to address these challenges, we introduce a framework in which model errors are captured by allowing variability in specific model components and parameterizations for the purpose of achieving meaningful predictions that are both consistent with the data spread, and can potentially disambiguate model and data errors. To achieve this, select existing or proposed model parameters are cast as random variables, representing model error, thereby casting the calibration problem within a density estimation framework. When parameters of the joint input density are difficult to estimate due to computational expense or degeneracy of exact likelihoods, we employ Approximate Bayesian Computation (ABC) to build prediction-constraining approximate likelihoods. We demonstrate the key strengths of the method on synthetic cases, as well as on two practical applications of interest, from chemical kinetics and atmospheric transport modeling.

Title: Turbulence During the Generation of Internal Waves at Rough, Underwater Topography

Author(s): Sutanu Sarkar, Masoud Jalali, *UC San Diego*.

The oscillating tide over rough, underwater topography launches internal gravity waves. These topographically generated waves constitute a key contributor to ocean turbulence during their generation, propagation through non-uniform stratification and reflection at solid boundaries. DNS and LES approaches allow high-resolution results for small-to-moderate scale model problems, thereby enabling the identification of nonlinear mechanisms that underlie the turbulent processes. We will discuss the dependence of turbulence levels and the associated dissipation rate on tidal forcing and topographic steepness.

Title: Seismic Response of Structural Models with Secondary Stiffness Capability

Author(s): Hamidreza Sarmadi, Lawrence Reaveley, *U. Utah.*

A novel concept of a multi-linear force-deformation model of a structural system that has a defined range of plastic behavior has been developed to be used in the next generation of structural seismic force resisting systems. This unique force-deformation behavior has been characterized with secondary stiffness and ductility which utilizes the traditional elasto-plastic system with additional behavioral characteristics. This enhanced elasto-plastic model has a secondary stiffness capability which is engaged after a specific amount of plastic deformation and follows by a secondary plastic deformation plateau. This unique structural system with secondary stiffness and ductility is noted a SSD. In addition to the exceptional characteristics of capacity force-deformation model of a SSD system, the secondary stiffness and ductility characteristics influence the seismic demand of the structural system by varying the stiffness, fundamental period and damping of the system. According to the theory underlying the model, it is postulated that, the structural cost of such a system may be reduced while providing enhanced performance as measured by limited drift and accelerations at various levels of a structure. Having a structural system that responds inelastically under small seismic loads may lead to more economical design. In this strategy, however, the safety of a structure experiencing higher levels of ground motion that are associated with infrequent large earthquakes becomes the main concern of the seismic design. Devices with secondary stiffness and ductility (SSD) can provide the required safety in higher seismic hazard levels while keeping the basic structural design economical. The seismic performance of the structural systems with the proposed force-deformation model has been investigated in this research. The comparison of structural responses for different structural systems such as a linear-elastic model, an elasto-plastic model, and a SSD model have used to show the capability of this novel and practical structural force-deformation model and the effects of the secondary stiffness and ductility characteristics. Single degree of freedom (SDoF) structures with the SSD models have been used to demonstrate the efficiency of the developed model through the controlled seismic responses using the numerical simulations. The OpenSees platform is enhanced to perform nonlinear time history dynamic analyses on nonlinear inelastic systems such as SSDs. The ground motion records, which incorporates the earthquake characteristics such as the source-to-site distance and soil type of the site are selected from the PEER NGA database and have been used for elastic-linear and inelastic-nonlinear time history analysis of the structural models. Results show the efficacy of the SSD force-deformation models in seismic response of structural systems under multi-level earthquake ground motions.

Title: Predicting the Rate of Dislocation-Precipitate Interactions with Atomistic Simulations

Author(s): Sepehr Saroukhani, Kelvin Leung, Derek Warner, *Cornell U.*; Linh Nguyen, *LLNL*; Chandra Singh, *U. Toronto*.

The high strength of many modern engineering alloys is attributed to the presence of microstructural obstacles to dislocation motion. The rate of overcoming each obstacle can be used to make important quantitative predictions and thus is a key step in understanding the plastic behavior of modern alloys. In this contribution, our focus is on the interaction between an edge dislocation with a GP-zone. The predictions from different variants of the Harmonic Transition State Theory (HTST), as the most common tool in the literature, are compared to those of direct Molecular Dynamics simulations. It is shown that these methods fail to provide accurate predictions as the problem has a large entropy barrier. Moreover, the performance of the Finite Temperature String (FTS) method as a tool for obtaining a reaction coordinate and computing the free energy profile for the Transition State Theory (TST) is discussed. It is shown that the problem has multiple reaction channels and FTS, although successful in identifying one of these channels, fails to provide a meaningful free energy profile. Finally, we show the Transition Interface Sampling (TIS) approach, which does not need a free energy profile and is known to be less reliant on the choice of reaction coordinate, is capable of providing close predictions to those of direct simulations.

Title: Arterial Wall Modeling with Time-Dependent Surface Extraction from Medical Images

Author(s): Takafumi Sasaki, Kenji Takizawa, Hirokazu Takagi, *Waseda U.*; Tayfun Tezduyar, *Rice U.*; Keiichi Itatani, Shohei Miyazaki, Kagami Miyaji, *Kitasato U.*

A method for coronary arterial dynamics computation with medical-image-based time-dependent anatomical models was introduced in [1]. One of the components of the method used in [1] was a curve-extraction technique [2], which was used in obtaining the time-dependent anatomical models from the medical images. The curve-extraction technique is based on minimizing the strain energy for a curved-beam representation of the artery, and from that the arterial model is constructed by associating time-averaged cross-sections to the points along the curve. Here we introduce a new method for arterial modeling from time-dependent medical images. We use a surface-extraction technique for obtaining the time-dependent anatomical model from the medical images. In this technique, the arterial surface geometry is extracted from the medical image by using a NURBS representation of the extracted surface, and the surfaces associated with different instants of the cardiac cycle all have a common parametric space. At each instant, the spatial control mesh is created by least-squares minimization of the difference between the NURBS representation of the surface and the surface coming from the medical image. The NURBS representation of the surface becomes the target geometry in the strain-energy minimization, and the resulting equations are solved over the arterial surface. We apply the method to a human aorta, with 20 medical images in the cardiac cycle. [1] K. Takizawa, R. Torii, H. Takagi, T.E. Tezduyar, and X.Y. Xu, "Coronary arterial dynamics computation with medical-image-based time-dependent anatomical models and element-based zero-stress state estimates", *Computational Mechanics*, 54 (2014) 1047-1053. [2] R. Torii, J. Keegan, N.B. Wood, A.W. Dowsey, A.D. Hughes, G.-Z. Yang, D.N. Firmin, S.A.M. Thom, and X.Y. Xu, "MR image-based geometric and hemodynamic investigation of the right coronary artery with dynamic vessel motion", *Annals of Biomedical Engineering*, 38 (8) (2010) 2606–2620.

Title: Micropolar Peridynamic Modeling of Quasibrittle Materials

Author(s): Nicolas Sau, Jose Medina, Ana Borbon, *U. Sonora*.

Quasibrittle structures subjected to loads that cause the formation and propagation of cracks exhibit a behavior where continuum mechanics is no longer applicable. In an effort to correct the shortcomings of continuum models, the peridynamic bond-based model was proposed in 2000. One of the shortcomings of the bond-based peridynamic model is that was not able to model materials with Poissons ratio different from 1/4 in three dimensions and 1/3 for plane stress problems. The micropolar peridynamic model improves the bond-based peridynamic model by allowing moment densities in addition to force densities to interact among particles inside the material horizon. A clear connection between the micropolar peridynamic model proposed in 2007 and continuum models was not fully established since stress tensor expressions were not incorporated. The stress tensor using the peridynamic theory was first introduced by Silling in 2000, and modified later by Lehoucq in 2008 to include the interaction between two volumes. In this work, it is proposed a framework where the micropolar peridynamic stress is developed, in which relationships between conventional stress-strain and the micropolar peridynamic stress-strain tensor for linear elastic materials are obtained. Using this framework, the stress tensor can be analyzed in regions where the displacement field is discontinuous. A numerical scheme for the calculation of the micropolar peridynamic stress was developed where results show convergence with classical linear elastic solutions for small values of the material horizon.

Title: Enriched Surface Finite Elements: A Simple Technique to Combine Isogeometric and Standard, Finite-Element Discretizations

Author(s): Roger Sauer, Callum Corbett, Raheel Rasool, *AICES, RWTH Aachen U.*

Recently a surface enrichment technique has been developed that combines isogeometric and standard finite element (FE) discretizations in order to exploit the advantages of both [1,2]. The key idea is to apply isogeometric analysis (IGA) to domains where higher accuracy and smoothness is required, while using efficient linear Lagrange finite elements in the rest of the domain. For this purpose various interface elements are developed - consisting of an IGA-enrichment of standard Lagrange FE - that enable the blending between isogeometric and standard FE discretizations. The enrichment technique is used equivalently for the discretization of the geometry and the unknown solution field. The technique is especially beneficial for problems governed by surfaces and interfaces, since in those problems the accuracy in a relatively small region can determine the overall accuracy. Initially, contact and debonding problems were studied [1,2], but the enrichment technique also extends to flow problems [3]. It is shown that the technique can increase robustness and accuracy, while being more efficient at the same time. The enrichment technique is rigorously compared with standard tri-variate Lagrange and isogeometric discretizations. It is further shown that the enrichment technique can also be used to simplify the generation of volumetric meshes from given IGA surface representations. The presented 3D numerical examples include frictional contact, mixed-mode debonding, incompressible flows and fluid-structure-interaction problems. References [1] C.J. Corbett, R.A. Sauer, NURBS-enriched contact finite elements, *Comput. Methods Appl. Mech. Engrg.* 275 (2014) 55–75. [2] C.J. Corbett, R.A. Sauer, Three-dimensional isogeometrically enriched finite elements for frictional contact and mixed-mode debonding, *Comput. Methods Appl. Mech. Engrg.* 284 (2015) 781–806 [3] R. Rasool, C.J. Corbett, R.A. Sauer, A strategy to interface isogeometric analysis with Lagrange finite elements - application to incompressible flow problems, in preparation

Title: A Comparison of Inverse Transformations for Elastodynamic Boundary Element Method

Author(s): Martin Schanz, *Graz U. Tech.*; Wenjing Ye, *Hong Kong U. Sci. & Tech.* ; Jinyou Xiao, *Northwestern Polytech'l. U.*.

Computing system responses due to transient forces can be made with the help of the Laplace or Fourier transform as long as the problem itself is linear. For linear elastodynamics, this is a convenient way to circumvent the CPU and storage intensive time domain Boundary Element (BE) formulations. For visco- or poroelasticity, it is even the only possibility due to missing time domain fundamental solutions. Unfortunately, the inverse transformation is still a task where experience in adjusting parameters is required. If a system without damping is considered, a normal Discrete Fourier Transfer (DFT) is insufficient and an artificial damping must be introduced. This results naturally to use the Laplace transform. The DFT combined with an exponential window method is such a technique. But for highly non-smooth signals, some windowing techniques (e.g., Blackman window) to smooth out the Gibbs oscillations produced due to the truncation of high frequency signals is necessary. Alternatively, the Convolution Quadrature Method (CQM) can be used. In contrast to the DFT approach in CQM only a suitable time step must be found. From an analytical point of view it can be shown that the DFT with the exponential window is similar to the CQM. Only the used complex frequencies differ. These similarities are presented and some studies of both methods for exemplary convolutions are performed. As well, BE computations are compared because both methods need different frequency calculations which may have different computing times. Finally, the results will be compared with respect to the overall efficiency to achieve a given error in time.

Title: Clinical Data-Aware Uncertainty Analysis of Multi-Scale Cardiovascular Models

Author(s): Daniele E. Schiavazzi, Justin S. Tran, Alison L. Marsden, *UC San Diego*; Giancarlo Pennati, *Politecnico di Milano*; Tain-Yen Hsia, *Great Ormond St. Hospital*; *UCL Inst. CV. Sci.*

The clinical impact of simulation tools in preventive care and surgical design is limited by the lack of measures of confidence typically associated with deterministic results. Despite the numerous sources of uncertainty affecting the results of these simulations (i.e., errors in clinical measurements of blood flow and pressures, uncertain vessel walls material properties and patient-specific anatomies), their effect on numerical simulation results has not been widely assessed in prior work. State-of-the art predictions of hemodynamics in patients are obtained through multiscale numerical modeling [1,2], where a three-dimensional SUPG finite element solver is coupled with an ODE circulation network, allowing a unified description of local and systemic circulation. When trying to characterize variability in the results of these models, classical assumptions of independence and identical distribution for random inputs may lead to an overestimation of the total system uncertainty, resulting in the need to infer these quantities directly from the available clinical measurements. Bayesian registration of multiscale cardiovascular models is also a particularly difficult task, due to the high dimensionality and non-linearity of ODE circulation models (leading to possible lack of identifiability and multimodal posterior) and due to the computational cost of iteratively solving a three-dimensional finite element model. In this context, we show that a multi-level approach to Bayesian registration can be used to enhance the ability of learning from the joint probability of the input parameters. Accordingly, prior distributions are updated from a preliminary sub-model analysis of the heart compartment, subject to prescribed aortic and venous flows. Improved convergence of Markov chain Monte Carlo approaches to stationary multimodal posteriors is also achieved using self-adaptive random sequences combining differential evolution and subspace sampling. Moreover, a pressure-flow rate surrogate is employed to minimize the computational burden during tuning. Finally, we consider the problem of propagating the uncertainty through multiscale models and discuss possible advantages of adopting forward propagation approaches promoting a sparse multiresolution representation for the stochastic model responses of interest. Examples focus on hemodynamics in single-ventricle physiology following Norwood surgery. [1] C.A. Taylor et al., Finite element modeling of blood flow in arteries, *Computer Methods in Applied Mechanics and Engineering*, 1998. [2] D.E. Schiavazzi et al., Hemodynamic effects of left pulmonary artery stenosis following superior cavopulmonary connection: a patient-specific multiscale modeling study, *The Journal of Thoracic and Cardiovascular Surgery*, 2015. [3] D.E. Schiavazzi et al., Sparse multiresolution regression for uncertainty propagation, *International Journal for Uncertainty Quantification*, 2014.

Title: Model-Order Reduction for Coupled Problems

Author(s): Wil Schilders, *TU Eindhoven*.

Coupled systems occur in many engineering applications, in particular in multi-physics problems. The coupling consists of the interaction, weak or strong, between different subsystems, described by different physical quantities such as temperature, structural mechanical displacements and electro-magnetic fields. After numerical discretization of the mathematical models of the coupled systems, the discretized systems are usually complex and of very large scale. This motivates the application of model order reduction techniques, intending to reduce the number of degrees of freedom, enable practical computation, and furthermore, significantly reduce the computational time. Model order reduction for coupled systems has been studied in structural dynamics since the 1960s, where a component mode synthesis (CMS) method was proposed [1]. In [2], the problem how to choose the important modes of the subsystems within CMS methods is addressed, and a moment-matching approach for choosing important modes is proposed. The CMS method builds upon the modal truncation method known in control and mechanical engineering, and in this sense, CMS belongs to modal truncation methods. Besides the CMS method widely used in structural dynamics, MOR methods based on systems and control theory like balanced truncation, and MOR methods based on approximation theory like moment-matching, as well as the MOR methods popular in mechanical engineering and fluid dynamics like the reduced basis method, proper orthogonal decomposition (POD), have been subsequently applied to coupled systems, and have achieved significant efficiency for various multi-physics problems. In this presentation, we discuss a new approach to the solution of coupled problems, based upon low rank approximations of the coupling blocks. The work is described in [3]. [1] W. C. Hurty. Vibrations of structural systems by component-mode synthesis. *Journal of the Engineering Mechanics Division (ASCE)*, 86:51–69, 1960. [2] B. S. Liao, Z. Bai, and W. Gao. The important modes of subsystems: A moment-matching approach. *International Journal for Numerical Methods in Engineering*, 70:1581-1597, 2007. [3] W.H.A. Schilders and A. Lutowska, A Novel Approach to Model Order Reduction for Coupled Multiphysics Problems, in: *Reduced Order Methods for Modeling and Computational reduction*, A. Quarteroni and G. Rozza (eds), Springer, pp. 1-50, 2014.

Title: Immersogeometric Analysis: The Role of Geometric Fidelity in Immersed Domain Finite Element Methods

Author(s): Dominik Schillinger, Vasco Varduhn, Lam Nguyen, Nickolaus Sundholm, *U. Minnesota*; Ming-Chen Hsu, Fei Xu, *Iowa State U.*

In this talk, we will first describe the concept of immersogeometric finite element methods, drawing on earlier work on the finite cell method. Influenced by isogeometric analysis, where the importance of eliminating geometric errors has gained broader recognition, the key feature of an immersogeometric method is the ability to faithfully represent the geometry of the immersed domain. We will illustrate with several examples that variationally consistent weak enforcement of boundary conditions and geometry-aware quadrature rules in intersected elements are the two key ingredients for high-fidelity immersed analysis. A significant advantage of immersed methods is their flexibility with respect to the underlying geometric model, from smooth boundary representations in computer aided geometric design to voxel representations obtained from medical imaging technologies. However, in the sense of the immersogeometric paradigm, the fidelity of the geometric model can significantly impact the accuracy level that is possible in image-based analysis. For example, we show that for phase-field fracture analysis crack initiation is extremely sensitive to the sawtooth pattern of the voxel data, even for image resolutions that are finer than the characteristic length scale of the diffusive crack. On the other hand, when image segmentation is not possible, voxel based simulations are the only option for patient-specific simulation. This is illustrated by CT scan based blood flow analysis through a capillary network with different flow regimes.

Title: Bijective Finite-Element Method

Author(s): Patrick Zulian, Rolf Krause, Kai Hormann, *U. Svizzera Italiana*; Teseo Schneider, *U.Svizzera Italiana*.

In a time-dependent non-linear elastic physical simulation a body is heavily deformed due to internal and external forces. The body is usually discretized by means of a mesh, and large deformations may lead to meshes with degenerate elements. Such degenerate elements might become flipped and have negative volume, which is unphysical, hence causing the simulation to stop. We propose a novel approach based on bijective maps which guarantees that the mesh does not degenerate. The main idea is to bijectively warp the mesh between two successive time steps. By doing so, we ensure that the elements will not flip and hence the simulation remains physical. In order to warp the mesh we employ the method proposed by Schneider et al. [1] which creates bijective maps between a source and a target polygon as composite mean value mappings. We extend the mapping not only to the vertices of the mesh but to the entire volume of the element, which also includes the edges, because otherwise the elements may flip due to the linearity of the edges. Since this leads to curved elements, we redefine all differential operators and propose a new way to exploit standard non-conforming domain decomposition techniques such as the L2-projection to transfer quantities from one deformed mesh to another. [1] T. Schneider, K. Hormann, M. S. Floater, Bijective composite mean value mappings, *Comput. Graph. Forum* 32 (5) (2013) 137-146.

Title: Fluid Structure Interaction Between Elastic Thin Shell and Multi-Phase Flow

Author(s): Kristianto Tjiptowidjojo, Andrew Cochran, *U. New Mexico*; P. Randall Schunk, *Sandia Nat'l. Lab.*

Fluid structure interactions in three-dimensional problems are typically handled via coupling between three-dimensional continuum representations of fluid and structural mechanics. However, when the problem of interest exhibits extreme dimensional aspect ratios, i.e., a disparate length scale such that the characteristic length of one dimension of the domain is much smaller than the others, this approach is often not practical. A more viable approach is to employ computational-shell-based reduced-order models of both fluid and structural mechanics. In this work, we develop a fluid-structure interaction model in very thin (sheet-like) geometries. Such geometries are often encountered in the manufacture of thin film coatings on flexible substrates, and more recently in nano-imprint lithography processes. Specifically, we derive and combine thin shell equations for both structures and multiphase flow. The thin shell model is a three-dimensional extension of that reported by Carvalho (2003), where we retain both membrane and bending resistance in the quasi static stress balance. The multiphase flow model is a coarse-grained extension of the multiphase lubrication flow model reported by Roberts et. al. (2013), but modified such that the liquid-gas interfaces are no longer tracked explicitly. We demonstrate the model's performance and effectiveness on a nano-imprint lithography process. References Carvalho, M. S.. Elastohydrodynamics of tensioned web roll coating process. *International Journal for Numerical Methods in Fluids* 2003; 41:561 – 576 Roberts, S. A., Noble, D. R., Benner, E. M., and Schunk, P. R.. Multiphase hydrodynamic lubrication flow using a three-dimensional shell finite element model. *Computers & Fluids*; 87:12 – 25

Title: Partition of Unity Methods: Fit for Industrial Use?

Author(s): Marc Alexander Schweitzer, *Fraunhofer SCAI & U. Bonn*; Albert Ziegenhagel, *Fraunhofer SCAI*.

We present the current state of the PaUnT software package which is a parallel implementation of a meshfree generalized finite element method based on the partition of unity approach. We show that the method and its implementation is stable and robust for arbitrary enrichment functions. PaUnT also comes with an efficient multilevel solver and a general variational mass lumping scheme applicable to arbitrary enrichments and higher order discretizations. Moreover, PaUnT provides a simple interface to couple it to commercial (and academic) finite element packages. We present results of large scale simulations of coupled PaUnT-FEM simulations from fracture mechanics, structural dynamics and fluid flow.

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Title: Complex Structural Assemblies of Weakly Continuous T-Splines

Author(s): Michael Scott, Kevin Tew, *Brigham Young U.*; Derek Thomas, *UT Austin*; John Evans, *U. Colorado-Boulder*.

In this talk we introduce a technique called weakly continuous geometry for the modeling of complex structural assemblies of T-splines where the non-manifold intersections can accommodate mismatched parameterizations and control meshes. Allowing for nonconforming interfaces dramatically simplifies the design process and/or isogeometric solution strategy for this class of problems. The resulting T-spline CAD representation, when used as a basis for isogeometric analysis, exhibits optimal convergence rates without any modification to the underlying finite element formulation. To build the underlying weakly continuous T-spline basis we employ Bézier projection. We demonstrate the efficacy of the approach for the design and analysis of complex structural assemblies of beams and shells and finite deformation solids.

Title: LES-SOMAR: An Adaptive Framework for Geophysical Simulations Across Multiple Scales

Author(s): Alberto Scotti, Edward Santilli, *UNC-CH*; Sutanu Sarkar, Vamsi Chalamalla, *UCSD*.

Geophysical flows are often characterized by a combination of marked anisotropy, different physical regimes (e.g., hydrostatic vs. non-hydrostatic), intermittence of turbulence and wide separation between the energy-containing scales and the turbulent scales where mixing and dissipation occurs. In this talk we will describe a computational framework for the evolution of non-hydrostatic, baroclinic flows encountered in regional and coastal ocean simulations. It combines the flexibility of Adaptive Mesh Refinement (AMR) with a suite of numerical tools specifically developed to deal with the high degree of anisotropy of oceanic flows and their attendant numerical challenges. The simulation is organized on a hierarchical grid. The base grid resolves the largest hydrostatic energy containing eddies. Finer grids can be embedded recursively to capture the finer scales that are generated once the base flow becomes unstable. The refinement can be either prescribed a priori in certain regions, or decided dynamically based on selected characteristics of the flow (e.g., vorticity magnitude). The embedded grids can be refined isotropically or anisotropically. The same solver is used across the tree, switching between hydrostatic to non-hydrostatic as the lepticity of the grid decreases. At the top-most level, the framework allows the insertion of a separate LES solver solved on a much finer grid, and two-way coupled with the solver on the lowest level. We will show some applications of this framework related to the generation of internal waves over topographic reliefs.

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Title: Transient Nearly/Fully Incompressible Elasticity with Simple Tetrahedral Finite Elements: A Variational Multi-Scale Approach

Author(s): Guglielmo Scovazzi, Xianyi Zeng, Simone Rossi, *Duke U.*; Brian Carnes, *Sandia Nat'l. Lab.*

A new tetrahedral finite element for transient dynamic computations of nearly and fully incompressible elasticity is presented. It utilizes the simplest possible finite element interpolations: Piece-wise linear continuous approximation for both the displacements and the pressure (hydrostatic) component of the stress tensor (P1/P1). The proposed method leverages a new type of variational multiscale stabilization, needed to stabilize the underlying Stokes operators associated with the linear and finite elasticity equations. Specifically, we pose the constitutive equation for the pressure in rate form rather than the canonical "static" form. It is shown in a number of computational tests that this modification is necessary in order to ensure stable computations in the transient dynamics case. To the knowledge of the authors, this represents a new finding in the theory of variational multiscale methods. An extensive suite of tests is presented to study the performance new method.

Title: Optimal High-Order, Strong-Stability-Preserving Linear Multi-Step Time Discretizations for Discontinuous Galerkin Methods

Author(s): Rachel Sebian, Ethan Kubatko, *Ohio State U.*; Ben Yeager, *Imperial College*.

Discontinuous Galerkin (DG) finite element spatial discretizations are often used in a method-of-lines approach with explicit time steppers for the numerical solution of hyperbolic conservation laws. Among the most widely used approaches of this category are the Runge-Kutta (RK) DG methods originally developed by Cockburn and Shu [1]. One of the oft-cited advantages of DG is the ease and efficiency with which high-order spatial accuracy can be achieved via the use of (local) high-degree polynomial spaces; however, in order to render the resulting (fully discrete) scheme high-order accurate, high-order time stepping methods that match the accuracy of the spatial discretization must be used [1]. Furthermore, proof of the total variation (TV) stability of these schemes requires the use of a special class of explicit time steppers known as strong-stability-preserving (SSP) methods. This, in effect, limits the order of RKDG methods to four due to the well-known order barrier of explicit SSP RK methods [2]. In this work, we explore the development and application of linear multistep (LM) DG methods as a means to overcoming this order barrier. Given that we employ explicit SSP LM methods, which have no order barrier, the resulting LMDG methods can (in theory) achieve any order of accuracy and inherit the proven TV stability properties of RKDG methods (albeit under different CFL conditions). Unfortunately, it was found that existing SSP LM methods have severe time step restrictions for linear stability when used with DG spatial discretizations. To remedy this, we constructed new SSP LM methods designed to achieve the maximum allowable time step that would maintain both linear and TV stability when used with DG spatial discretizations. Our new methods exhibit impressive efficiency improvements over the existing SSP LM methods and more important, allow us to efficiently surpass the fourth-order barrier of RKDG methods. We demonstrate the stability and convergence properties of the resulting LMDG methods in a series of numerical tests and conclude by discussing future work in this area that aims for further improvements through the use of multistep, multistage SSP methods. References [1] B. Cockburn and C.-W. Shu. Runge-Kutta Discontinuous Galerkin Methods for convection-dominated problems. *Journal of Scientific Computing*, 2001. [2] S. Gottlieb, D. Ketcheson, and C.-W. Shu. *Strong Stability Preserving Runge-Kutta and Multistep Time Discretizations*. World Scientific, 2011.

Title: Computational Micromechanics-Based Exploration of Strain and Damage Sensing Capabilities in CNT-Polymer Nanocomposites

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

The finite elements based 2-scale computational multiscale micromechanics based exploration of strain and damage sensing capabilities in carbon nanotube (CNT)-polymer nanocomposites focuses on the macroscale piezoresistive response when the nanocomposite is subjected to monotonic and cyclic loading conditions. It has been shown that electron hopping at the nanoscale is the primary mechanism behind the observed macroscale piezoresistivity for such nanocomposites. A novel continuum description of the non-continuum electron hopping effect used in the current work enables the use of multiscale continuum micromechanics based approaches to study nanocomposite piezoresistivity. In addition to the deformation based piezoresistive response, the effect of interfacial damage and local matrix damage at the nanoscale has been studied in the current work. Interfacial separation/damage is allowed at the nanoscale CNT-polymer interface using electromechanical cohesive zones to account for electron hopping across the separated interface. The mechanical response of the CNT-polymer interface is obtained in terms of normal/tangential traction-separation behavior from atomistic scale Molecular Dynamics based models. The coupled electrostatic response is based on evolving interfacial resistance through the electron hopping induced current density across the separated interface. It is observed that the effective macroscale piezoresistive response obtained from the current modeling framework captures interfacial separation/damage state and shows sensitivity to damage accumulation over several cycles. Local matrix damage at the nanoscale has been modeled at the nanoscale using Continuum Damage modeling. For the progressive continuum damage in the polymer matrix, the Christensen's failure criterion is applied for damage initiation, with a phenomenological damage law used for damage evolution. It is observed that local matrix damage can be closely correlated to diminishing intertube conductive paths at the nanoscale leading to effective piezoresistive response. Furthermore, to better understand the correlation of the macroscale piezoresistive response with the CNT dispersion at the microscale, a 2-scale concurrent computational multiscale micromechanics model is constructed to predict the effective macroscale piezoresistive response of CNT/polymer nanocomposites. Several different microscale dispersion architectures are studied. The results obtained from the concurrent 2-scale analysis give reasons and provide bounds for the wide range of gauge factors found in the literature offering insight regarding how control of the microscale CNT networks can be used to tailor nanocomposite piezoresistive response. Such exploration of the governing physical mechanisms starting at the smallest scale of influence and transitioning into macroscale effective properties provides key insights into the multiscale problem.

Title: A Stabilized Lagrange Multiplier Formulation for an Inverse Elasticity Problem Formulated as a PDE Constrained Optimization Problem

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

Inverse problems with interior data arise in a variety of applications, such as: aquifer management, non-destructive testing, and elasticity imaging. Iterative approaches to their solution involve casting the inverse problem as a constrained optimization problem where the function to be minimized contains data-matching and regularization terms, and is constrained to satisfy a governing system of PDEs. The adjoint method described in (1) solves the problem by repeating four steps: (i) Solve a forward problem for the state variables given a current iterate of the material parameters; (ii) solve an adjoint problem for the dual variables; (iii) use the products of steps one and two to evaluate the objective function and its gradient; (iv) utilize these to update the material parameters for the next iteration. The forward and adjoint problems require complete sets of boundary conditions to be well-posed. In many inverse problem applications, however, these boundary conditions are poorly characterized or even entirely unknown. For example, in ultrasound elasticity imaging applications (2,3), confidence is high in only one of the measured displacement components, while uncertainty is high in the others. As a result, without additional input of information, the boundary conditions required for the forward and adjoint problems are poorly characterized, which leads to unnecessary error in the inverse problem solution. We propose a stabilized Lagrangian formulation of the inverse problem that assumes no boundary conditions and thus removes their undue influence from the problem's solution. This formulation has the drawback that the forward and adjoint problems do not decouple; therefore, we solve for the state and Lagrange multiplier variables simultaneously. We include a GLS term to enhance stability of the PDE constrained optimization problem. Results obtained from the application of this formulation to both simulated and experimental ultrasound elasticity imaging data will be presented. References: 1. Oberai, Assad A., Nachiket H. Gokhale, and Gonzalo R. Feijóo. "Solution of inverse problems in elasticity imaging using the adjoint method." *Inverse Problems* 19.2 (2003): 297. 2. Doyley, M. M. "Model-based elastography: a survey of approaches to the inverse elasticity problem." *Physics in medicine and biology* 57.3 (2012): R35. 3. Parker, K. J., M. M. Doyley, and D. J. Rubens. "Imaging the elastic properties of tissue: the 20 year perspective." *Physics in medicine and biology* 56.1 (2011): R1.

Title: Improving Finite Volume Methods Through Better Reconstruction

Author(s): Chandan Sejkan, Carl Ollivier-Gooch, *U. British Columbia Vancouver.*

One goal of CFD is to reduce the numerical error in the computed solution. For finite volume schemes, this error originates as error in the flux integral. For diffusion problems on unstructured meshes, the flux (computed from reconstructed gradients) is one order less accurate than the reconstructed solution. Worse, the gradient errors are not smooth, and so no error cancellation accompanies the flux integration, reducing the flux integral to zero order for the second order schemes. Our aim is to compute the gradient and flux more accurately at the cell boundaries and hence obtain a better flux integral for a slight increase in computational costs. We propose a novel reconstruction method and also a distance-weighted gradient averaging scheme to improve flux accuracy for second-order accurate discretization of diffusion on cell-centered, isotropic unstructured meshes. Our approach uses a modified least squares system to reconstruct the solution to second order accuracy in the H_1 norm instead of the prevalent L_2 norm, thus ensuring second-order accurate gradients. Circumcenters are chosen as the cell reference points to facilitate calculation of second order gradients at flux quadrature points using a distance-weighted averaging scheme. The distance-weighted scheme is robust enough to accommodate cells whose circumcenters lie outside the cell. Our results show a significant improvement in the order of accuracy of the computed flux as well as the flux-integral. When applied to a channel flow advection-diffusion problem, the scheme resulted in an increased order of accuracy for the flux integral along with gains in solution accuracy by a factor of two. These gains are primarily from our implementations in the diffusive flux calculation and hence are influenced by the coefficient of diffusion used in the advection-diffusion problem. However, for pure Poisson cases we have observed that the scheme shows some instability. The eigenvalue analysis tool proposed by Jalali et al. [1] was used to visualize the stability of the scheme and it was found that the scheme has a form of odd-even solution decoupling similar to that seen in regular L_2 reconstruction on structured meshes. This instability can be mitigated with the introduction of a jump term, but doing so adversely affects the accuracy gains. Work is in progress to counter these instabilities. [1] Jalali A, Sharbatdar M, Ollivier-Gooch C. Accuracy analysis of unstructured finite volume discretization schemes for diffusive fluxes. *Computers & Fluids* 2014;101:220-232.

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Title: Convergence Studies of Meshfree Peridynamic Simulations

Author(s): Pablo Seleson, *Oak Ridge Nat'l. Lab.*; David Littlewood, *Sandia Nat'l. Lab.*.

The peridynamics theory of solid mechanics is a nonlocal reformulation of the classical continuum mechanics theory, suitable for material failure and damage simulation. A meshfree approach for the discretization of governing equations is the most widely discretization method used in peridynamics to date, due to its implementation simplicity and relatively low computational cost. This approach exhibits, however, accuracy and convergence issues in numerical solutions of peridynamic problems. In this talk, we will discuss those issues and present improvements in the accuracy and convergence of numerical solutions of meshfree peridynamic simulations, through the use of enhanced quadratures and smoothly decaying influence functions.

Title: Multi-Scale Modeling of the Interaction of a Shock Wave with a Particle-Laden Gas Using Metamodeling Techniques

Author(s): Oishik Sen, H.S. Udaykumar, *U. Iowa*; Sean Davis, Gustaaf Jacobs, *San Diego State U.*

In a typical multiscale modeling problem, information needs to be transferred across disparate length scales. Consider the problem of a shock wave passing through a gas laden with solid particles [1]. The particle scale (of the order of microns) is governed by meso-scale conservation equations for each of the solid and fluid phases[1] separately, while on the other hand the system scale (of the order of meters) is governed by macro-scale conservation equations which average over the solid and fluid phases[2]. This averaging process results in source terms in the macro-scale governing equations, e.g. particle drag etc. Typically such source terms are obtained from empirical models constructed from physical experiments. Not only are the experiments expensive, but also such experiments can only be performed in a limited parameter space (e.g. particle volume fraction, shock strength etc), which may be vastly different from the shock strength, volume fraction etc encountered by the particles in the actual macro-scale. The current research demonstrates the use of high-resolution meso-scale computational experiments which serve as surrogates to physical experiments in constructing the aforementioned source terms. The novelty of such an approach is that the computational experiments can be designed on a parameter space that is of relevance to the meso-scale. In the current work, a massively parallel computational code, SCIMITAR3D is used to perform [1] the meso-scale computations. The research further demonstrates the efficient use of metamodels to “lift” the relevant information from the mesoscale to the macro-scale equations; the meso-scale simulations provide a numerical drag law which can be readily used as a source term in macro-scale governing equations. Finally, this numerical drag law is used in an Eulerian-Lagrangian macro-scale code [2] to study shock interactions with particle curtains in shock tubes and the results are compared with experimental data in such systems. References: 1.Lu C, Sambasivan S, Kapahi A, Udaykumar HS. Multi-scale modeling of shock interaction with a cloud of particles using an artificial neural network for model representation. IUTAM Symposium on Linking Scales in Computations: From Microstructure to Macro-scale Properties 2012; 3:25–52. 2.Jacobs Gustaaf B, Don Wai-Sun. A high-order WENO-Z finite difference based particle-source-in-cell method for computation of particle-laden flows with shocks 2009; 228:1365-1379.

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Title: A High-Order, Space-Time Formulation for Non-Linear Structures with Applications to Coupled Multiphysics Applications

Author(s): Padmanabhan Seshaiyer, *George Maon U.*; James Cameron, *George Mason U.*; Saroja Erabelli, *MIT*.

Several multi-physics applications from engineering employ models for non-linear structures such as beams, plates or shells as fundamental structural elements. Some examples include modeling aero-elastic problems, robotic applications, and offshore structures. In this work, we study the dynamics of non-linear structures that often arise in coupled multi-physics applications. In particular, we consider dynamic nonlinear Euler–Bernoulli beam equations that are solved via a high-order finite element method in space and a high-order continuous formulation in time. Stability results are established for the mathematical model of the beam developed that is non-linear in geometry as well as influenced by temperature. Numerical results using the high-order space-time formulation are also presented that helps predict the dynamics of the non-linear structure efficiently. Our results suggest that the high-order space and time formulation presented herein is robust and can be applied to related benchmark applications.

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Title: A Fully-Coupled, Finite-Element/Finite-Volume Approach to Hydraulic Fracture Simulation for Massively Parallel Simulations

Author(s): Randolph Settghost, Joshua A. White, Pengcheng Fu, Stuart D.C. Walsh, Mike Puso, Joseph P. Morris, *LLNL*.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. This document is LLNL report LLNL-CONF-664703. The simulation of hydraulically driven fracture propagation presents significant challenges. In this work, the authors present a fully coupled method that applies the Finite Element Method to body deformations, and the Finite Volume Method to the flow of fluid through the fracture and rock matrix. We discuss challenges associated with the Finite Element/Finite Volume approach, and outline techniques to avoid singularities, and improve the poorly conditioned systems that result from this approach through modifications to the governing equations. In addition, methods for massively parallel strategies for solution of the non-linear systems that result from this approach will be discussed. Verification studies are presented for simple cases and compared with analytical solutions, and validation with lab scale experiments are presented.

Title: Solution of Eulerian Frame MHD Simulations with Multi-Stage RK Implicit/Explicit (IMEX) Time Integration

Author(s): John Shadid, Eric Cyr, Roger Pawlowski, *Sandia Nat'l. Lab.*

The magnetohydrodynamics (MHD) model describes the dynamics of charged fluids in the presence of electromagnetic fields. The mathematical basis for the continuum modeling of these systems is the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and energy, augmented by the low-frequency Maxwell's equations. This PDE system is non-self adjoint, strongly-coupled, highly-nonlinear, and characterized by physical phenomena that span a very large range of length- and time-scales. To enable accurate and stable approximation of these systems a range of spatial and temporal discretization methods are commonly employed. In the context of finite element spatial discretization methods these include mixed integration, stabilized methods and structure-preserving (physics compatible) approaches. For effective time integration for these systems some form of implicitness is required. Two well-structured approaches, of recent interest, are fully-implicit and implicit-explicit (IMEX) type methods[1,2]. This talk considers the initial evaluation of IMEX - Runge Kutta (RK) type methods for Eulerian frame simulation of challenging MHD systems. In this context issues related to stability, order-of-accuracy, and relative-accuracy are considered by numerical evaluation of the methods and comparison with fully-implicit multi-stage (RK) and multi-step (backward-differentiation, BDF) type methods. In this specific study for the semi-discretization in space, a residual-based variational multiscale (VMS) formulation for resistive MHD is employed [3]. Results for verification, benchmark, and challenging MHD application problems are presented. These include MHD duct-flows, driven magnetic reconnection in the island coalescence problem, simplified tearing-mode simulations, and hydromagnetic Kelvin-Helmholtz shear layers. [1] L. Pareschi and G. Russo. Implicit-explicit Runge-Kutta schemes and applications to hyperbolic systems with relaxation, *Journal of Scientific Computing.*, 25(112):129–154, 2005. [2] W. Hundsdorfer and S. J. Ruuth, Imex extensions of linear multistep methods with general monotonicity and boundedness properties, *J. Comp. Phys.* , 225:2016 – 2042, 2007. [3] J. N. Shadid, R. P. Pawlowski, E. C. Cyr, R. S. Tumiaro, P. D. Weber, L. Chacon, Scalable Implicit Incompressible Resistive MHD with Stabilized FE and Fully-coupled Newton-Krylov-AMG, submitted to CMAME

Title: Towards Modeling of Failure in Polycrystalline Ti Alloys Under High Rate of Deformation Using Crystal Plasticity FEM

Author(s): Ahmad Shahba, Xiaohui Tu, Somnath Ghosh, *Johns Hopkins U.*

Understanding failure of titanium alloys and developing high fidelity failure models for these alloys are of paramount importance due to their numerous applications ranging from biomedical devices to automobile and military industries. Failure of these alloys under extreme conditions, high rate of deformation specifically, is attributed to strain localization in narrow micron-size bands, namely adiabatic shear bands (ASBs) [1]. The failure of these alloys is culminated by nucleation and propagation of micro-cracks along the ASBs. Clearly temperature increase due to adiabatic heating and the resulting thermal softening play major roles in failure of these alloys. It is worthy to note that adiabatic heating is dictated by the local plasticity occurring in grain scale. Proper failure analysis of Ti alloys obviously requires one to incorporate in the model micro- scale features including both morphological and crystallographic properties. In this respect, crystal plasticity FEM (CPFEM) is an appropriate powerful tool for failure analysis as it enables one to capture the effects of microstructural details. In order to quantify the plasticity due to dislocation glide on different slip systems, Orowan's equation is employed which expresses the plastic shear strain rate in terms of average dislocation velocity. In this work, a new formulation is proposed for average dislocation velocity which is applicable for a wide range of strain rates and temperature. This average dislocation velocity formulation is informed by both thermally-activated and drag-dominated processes which govern dislocation motion under low and high levels of stress, respectively. Such a temperature-dependent CP framework is advantageous as it could be used in high rate simulations effectively where the adiabatic heating is of high importance in failure modeling. Moreover, the CP laws are developed in terms of dislocation densities to carry out a deformation-mechanism-based constitutive modeling rigorously. In this work, we try to understand how adiabatic heating and thermal softening are governed by the microstructural features and how thermal effects lead to shear localization in the microstructure. References [1] F. Martinez, LE. Murr, A. Ramirez, MI. Lopez, SM. Gayton, Dynamic deformation and adiabatic shear microstructures associated with ballistic plug formation and fracture in Ti-6Al-4V targets, *Materials Science and Engineering A* 454-455 (2007) 581-589

Title: Bayesian Calibration of Reaction Rate Model Parameters in Reacting Multiphase Flow Simulations for Advanced Coal Gasifier Technology Development

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 (DOE) continues to have great interest in technologies that reduce the CO₂ emissions of coal based power plants. Advanced power generation processes such as the Integrated Gasification Combined Cycle (IGCC) support this initiative by converting coal into synthesis gas (syngas) while capturing CO₂ for storage thereby reducing the environmental impact of power generation. Advanced modeling and simulation capabilities aim to reduce the cost and time to market of new energy technologies like IGCC by reducing costly design and scale-up testing. The DOE National Energy Technology Laboratory (NETL) recently launched uncertainty quantification (UQ) initiative to explore the applicability of available UQ techniques and open-source toolboxes in assessing uncertainties in gasification simulations. The first phase of this initiative focused on forward propagation of input uncertainties via traditional non-intrusive UQ methods. In the second phase, non-intrusive Bayesian calibration and UQ methods (in particular GE's Bayesian Hybrid Modeling framework, GEBHM [1]) were employed for the same gasifier configuration where extensive experimental data was also available. This talk will be focusing on the results of the second phase, where Optimal Latin Hypercube sampling was performed on a computational fluid dynamics (CFD) model of the fluidized bed gasifier with the open-source code MFIX [2]. In addition to the 3 input factors varied during the experiments, an additional modeling parameter (Arrhenius rate pre-exponent multiplier) was considered for Bayesian calibration. Several quantities of interest (CO, CO₂, H₂ species mole fractions at the exit) were modeled using GEBHM as Gaussian Processes. Since reacting multiphase flows are complex by nature and require transient simulations due to non-linearities, the computational resource requirements for acceptable time-to-solution are prohibitively expensive, which makes the sampling methodology and sample size critical components in the overall UQ effort. To be conservative, thirty sampling simulations were performed at one of the national leadership computing facility as part of the ASCR Leadership Computing Challenge (ALCC) award allocation. Results of the GEBHM UQ analysis will be presented for the calibration parameter, which previously used to be fixed and set in the CFD simulations in ad-hoc manner. In addition, global sensitivity and discrepancy analysis results from GEBHM will also be presented. The use of this additional sensitivity information to guide the design process will be discussed. References: 1. Kumar, N., et al., "Improving High-Dimensional Physics Models Through Bayesian Calibration with Uncertainty Data," TurboExpo, 2012, Copenhagen, DK. 2. MFIX, URL: <https://mfix.netl.doe.gov>

Title: Atomistic Simulation of Initiation in Hexanitrostilbene

Author(s): Tzu-Ray Shan, Aidan Thompson, Ryan Wixom, Cole Yarrington, *Sandia Nat'l. Lab.*

We report on the effect of cylindrical voids on hot spot formation, growth and chemical reaction initiation in hexanitrostilbene (HNS) crystals subjected to shock loading. Large-scale, reactive molecular dynamics simulations are performed using the reactive force field (ReaxFF) as implemented in the LAMMPS software. The ReaxFF force field description for HNS has been validated previously by comparing the isothermal equation of state and Hugoniot to available diamond anvil cell (DAC) measurements and density function theory (DFT) calculations and by comparing the primary dissociation pathway to *ab initio* calculations. Micron-scale molecular dynamics simulations of a supported shockwave propagating through the HNS crystal along different principal orientations are performed with an impact velocity (or particle velocity) of 1.25 km/s, resulting in shockwave propagation at ~4.4 km/s in the bulk material and a bulk shock pressure of ~2.5 GPa. The effect of cylindrical void sizes varying from 0.02 to 0.1 micrometers on hot spot formation and growth rate has been studied. Interaction between multiple voids in the HNS crystal and its effect on hot spot formation will also be addressed. Results from the micron-scale atomistic simulations are compared with hydrodynamics simulations.

Title: Adaptive Reconnection-Based Arbitrary Lagrangian Eulerian Methods

Author(s): Mikhail Shashkov, *XCP-4, LANL*.

We present a new adaptive reconnection-based Arbitrary Lagrangian Eulerian methods - ReALE methods. The main elements in a standard ReALE method, [1], are: An explicit Lagrangian phase on arbitrary polygonal mesh in which the solution and positions of grid nodes are updated; a rezoning phase in which a new grid is defined - number of mesh cells in rezoned mesh is {\em not changing}, but the connectivity of the mesh is allowed to change (it is based on using Voronoi tessellation; and a remapping phase in which the Lagrangian solution is transferred onto the new grid. In standard ReALE method rezoned mesh is smoothed by using one or several steps toward centroidal Voronoi tessellation, but it is not adapted to the solution in any way. In current paper we present two adaptive ReALE methods. Both methods are based on following design principles. First, it is using monitor (error indicator) function based on gradient or Hessian of some flow parameter(s), which is measure of interpolation error. Second, using equidistribution principle for monitor function as criterion for creating of adaptive mesh. Third, using weighted centroidal Voronoi tessellation as a tool for creating adaptive mesh. Fourth, we modify raw monitor function - we scale it to avoid very small and very big cells and smooth it to create smooth mesh and allow to use theoretical results related to weighted centroidal Voronoi tessellation. In first method - R-ReALE (R stands for Relocation) - number of mesh cells is chosen at the beginning of the calculation and does not change with time, but mesh is adapted to modified monitor function at rezone stage at each time step. In second method - A-ReALE (A stands for Adaptive) - both number of cells and their locations allowed to change at rezone stage on each time step. The number of generators is chosen to guarantee required spatial resolution where the modified monitor reaches its maximum value. We present all details required for implementation of new adaptive ReALE methods and demonstrate their performance in comparison with standard ReALE method. on series of numerical examples. [1] R.Loubere, P.-H. Maire, M.~Shashkov, J.~Breil, and S.~Galera. ReALE: A Reconnection-based Arbitrary-Lagrangian-Eulerian method. *Journal of Computational Physics*, 229(12):4724 -- 4761, 2010.

Title: Towards Computational Diagnosis of Coronary Artery Disease

Author(s): Simon Shaw, *Brunel U.*

Blood flow past stenoses in atherosclerotic coronary arteries may, within a range of percentage lumen occlusions, be accompanied by a 50-500 Hz acoustic signal - or 'bruit' - that manifests at the chest wall. The detection and localization of this very weak signal has the potential, [1] for example, to provide a low-cost and non-invasive technology that could be deployed as a routine screening device for atherosclerosis, or even as a diagnostic tool for treatment 'stratification' prior to the involvement of more expensive staff and equipment. This presentation will describe an early stage proof-of-concept investigation into using computational mathematics, underpinned by experimental verification, to prototype such a device. We describe an in-vitro rig of cylindrical tissue mimicking agarose gel through which a simulated stenosis signal is transmitted, under reproducible conditions, from its central bore to its surface. We describe a time domain finite element forward solver that simulates this rig and an inverse solver that, given the surface signal, attempts to localise its source. We will explain current progress in obtaining the viscoelastic properties of the gel using both direct experimentation for the static values and an inverse method, [2], for the time constants. Our long term aim is an inexpensive tool that, given the chest surface signal, can non-invasively diagnose the presence of coronary artery disease. Our scaled down axisymmetric homogeneous 'virtual chest' will be described in some detail and an illustrative - and encouraging - set of localisation results will be given both with and without simulated noise on the measured signals. This work was supported in the UK by the Engineering and Physical Sciences Research Council under grants: EP/H011072/1 & EP/H011285/1. [1] J Semmlow and K Rahalkar, Acoustic Detection of Coronary Artery Disease. *Annu. Rev. Biomed. Eng.*, 9:449-69, 2007. [2] HT Banks, S Hu, ZR Kenz, C Kruse, S Shaw, JR Whiteman, MP Brewin, SE Greenwald, M Birch. Model validation for a noninvasive arterial stenosis detection problem. *Math. Biosci. Eng.*, 11:427-448, 2014.

Title: A Hybridizable Discontinuous Galerkin Formulation for Fluid-Structure Interaction

Author(s): Jason Sheldon, *Penn. State U.*

Current generation tools for fluid-structure interaction (FSI) simulations are insufficient for fully-coupled problems of practical importance due to poor computational scaling for higher-order calculations and poor computational efficiency. A potentially better technique is the hybridizable discontinuous Galerkin (HDG) method, which was developed by Cockburn et al. [1] to overcome the main criticism of discontinuous Galerkin methods: high computational cost. By hybridizing the unknowns into local element unknowns and global element interface unknowns, HDG reduces the number of globally coupled unknowns, along with computational cost, while preserving accuracy. It also preserves the good scaling for high-order calculations possessed by discontinuous Galerkin methods, which will be crucial for high-order calculations of practical FSI problems. To date, applications of the HDG method have been limited in scope to non-multi-physics scenarios such as elastodynamics [2] and Navier-Stokes [3] problems; however, all of the components necessary for HDG FSI are present and the largest remaining hurdle is coupling them together. We present our preliminary work towards the realization of a hybridizable discontinuous Galerkin finite element method for monolithically coupled fluid-structure interaction. HDG formulations are presented for linear elastostatics for mesh motion, dynamic hyperelasticity for the solid, and arbitrary Lagrangian-Eulerian Navier-Stokes for the fluid. These are then combined into a monolithically coupled FSI formulation. We present verification of these individual components through the method of manufactured solutions, results for example problems solved with the individual components, and finally some preliminary HDG FSI results. We conclude by discussing our ongoing research plan for the future. Some of the areas we plan to explore are effects from variation of the stability parameter, difficulties in turbulence modeling for high Reynolds number flow, potential challenges for massively parallel simulations, and comparison with other FSI methods (e.g., partitioned coupling, continuous Galerkin, etc.). Determining conditions where the most computationally efficient method is HDG FSI is of particular interest. [1] B. Cockburn and J. Gopalakrishnan. New hybridization techniques. *GAMM- Mitteilungen*, 2:154–183, 2005. [2] N. C. Nguyen, J. Peraire, and B. Cockburn. High-order implicit hybridizable discontinuous Galerkin methods for acoustics and elastodynamics. *Journal of Computational Physics*, 230(10):3695–3718, 2011a. [3] N. C. Nguyen, J. Peraire, and B. Cockburn. An implicit high-order hybridizable discontinuous Galerkin method for the incompressible Navier–stokes equations. *Journal of Computational Physics*, 230(4):1147–1170, 2011b.

Title: Phase Field Formulation for Brittle Fracture in an Euler-Bernoulli Beam

Author(s): Yongxing Shen, Jian Gao, *Shanghai Jiao Tong U.*

The advantage of the phase field method for fracture is that the cracks are a natural outcome of numerical computation and requires no explicit tracking of the crack paths. Such idea has been generalized to structural elements such as shells [1]. In [1], the phase field is assumed constant across the thickness, thus only allowing complete fracture in the thickness and precludes fracture by bending. In this work we present a phase-field model to simulate brittle fracture in an Euler-Bernoulli beam. We start from formulating the problem with the principle of minimum potential energy in a 3D solid, with the displacement field and the phase field as primary arguments. We then select, for each cross section, representative fields that characterize the said cross section, including the beam deflection and rotation, and up to three quantities that represent the phase field within the cross section. The problem then reduces to a one-dimensional nonlinear differential equation and can be solved with the finite element method. A feature of the proposed method is, without discretizing the phase field within the cross section, it can represent its variation within the cross section, allowing to simulate fracture due to bending as well as axial loads. [1] F. Amiri, D. Millan, Y. Shen, T. Rabczuk, and M. Arroyo. Phase-field modeling of fracture in linear thin shells. *Theoretical and Applied Fracture Mechanics* 69 (2014) 102–109.

Title: Using Fracture Toughness Tests in a Multi-Scale Modeling Framework for Application to Concrete Penetration/Perforation Modeling

Author(s): Jesse Sherburn, William Heard, Omar Flores, Catherine Stephens, Michael Hammons, *US Army Engineer Rsch. & Dev. Center.*

The military and civil communities have keen interest the responses of structures to extreme loading environments. Numerical modeling of these extreme loading environments is especially challenging when applied to heterogeneous materials like concrete. In some loading conditions, such as penetration and fragmentation, the traditional finite element method is not effective in modeling the loading event in concrete unless significantly modified. One approach to model the heterogeneity of concrete is to rigorously model a small sample of the material at sub-scale and use the response and damage information in the less detailed full-scale model. The work by Ren et al. [1] introduced a framework known as the micro-crack informed damage model, which employs a multiscale approach to modeling damage in concrete. This approach first solves for the microscale using a microcell analysis and uses an energy-bridging technique to create a damage evolution law for the continuum scale analysis. The microcell calculations allow explicit cracks and voids to be included allowing the heterogeneous nature of concrete to be captured. The objective of this study is to obtain fracture toughness data and use that data to perform microscale calculations to determine a continuum scale damage evolution law. Additionally, lab-scale penetration/perforation experiments are conducted and appropriately modeled as an application of the developed damage evolution law. In this study a new concrete material is introduced and fracture toughness tests are conducted. The reproducing kernel particle method (RKPM), which requires fracture toughness as an input parameter, is used to solve the microscale calculations to determine a continuum scale damage evolution law. RKPM is used again to model the continuum-scale penetration/perforation problem, which has been previously been demonstrated by Guan et al. [2].

References [1] X. Ren, J.S. Chen, J. Li, T.R. Slawson, M.J. Roth, Micro-cracks informed damage models for brittle solids. *International Journal of Solids and Structures*. 48, 1560-1571, 2011. [2] P.C. Guan, S.W. Chi, J.S. Chen, T.R. Slawson, M.J. Roth, Semi-Lagrangian reproducing kernel particle method for fragment-impact problems. *International Journal of Impact Engineering*, 38, 1033-1047, 2011. * Permission to publish was granted by Director, Geotechnical and Structures Laboratory.

13th U.S. National Congress on Computational Mechanics
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Title: Quantitative, Elastoplastic Phase-Field Model for Solid State Phase Transformation Under Stress and Temperature Gradients

Author(s): San-Qiang Shi, *Hong Kong Polytech. U.*

Quantitative prediction of three-dimensional microstructure evolution during phase transformation in solids is often very challenging, especially when stress, composition and temperature gradients are present, together with plastic deformation. This paper takes hydride precipitation in zirconium alloys and void growth in irradiated metals as examples and shows how it could be done in nano-, micro, meso- and macro-scales within phase-field scheme. In recent years, the author's research team has developed a phase-field scheme to simulate the morphological and microstructural evolution of hydride precipitation in single and polycrystalline zirconium under uniform and non-uniform stress and temperature fields. Recent effort was devoted to develop a quantitative model for hydride precipitation and void growth. The model for hydrides takes into account crystallographic variants of hydrides, interfacial energy between hydride and matrix, interfacial energy between hydrides, elastoplastic hydride precipitation and interaction with externally applied stress and/or temperature field. The model for hydrides and for void are fully quantitative in real time and real length scale, and simulation results were compared with limited experimental data available in the literature with a reasonable agreement. However, some numerical and physical issues remain to be solved. This work was supported by grants from Research Grants Council of Hong Kong (PolyU 5267/10E) and the Natural Science Foundation of China (No.51271157).

Title: Adjoint-Based Mesh Adaptation for the 3D Navier-Stokes Equations

Author(s): Lei Shi, Z.J. Wang, *U. Kansas.*

With continuous progresses in numerical methods and computer hardware over the past several decades, Computational Fluid Dynamics (CFD) is now used routinely as a powerful tool in the design of aircraft. As it is still too expensive to obtain mesh-independent simulations in 3D, design computations still rely heavily on the experience of CFD users to generate results of “engineering accuracy”. In this paper, we developed a robust and efficient CFD framework for compressible Navier-Stokes equations that can provide engineering accuracy with little user interference by relying on two key components: efficient high-order CFD methods and automated mesh adaptation with a reliable error estimation. Current production CFD codes used in the aerospace industry are usually second order accurate, while 3rd and higher order ones are called high-order methods in the aerospace community. Because of their considerable potential, high-order methods have received significant research interest in the global CFD community in the last two decades. A variety of high order methods have been developed. In the current study, we focus on developing an adjoint-based mesh adaptation strategy for a recent nodal differential high-order formulation named the correction procedure via reconstruction (CPR). This formulation is easy to understand, efficient to implement and can recover several well known methods such as the discontinuous Galerkin (DG), the spectral volume method (SV) and the spectral difference methods (SD). Solution-based adaptive approaches are capable of dynamically distributing computational resources to desired regions to achieve required accuracy with minimum cost and user interference. They have been successfully demonstrated for a wide variety of applications, including the finite volume and DG methods. The effectiveness of adaptive methods highly depends on the accuracy of the error estimation and the adaptation criteria. Adjoint-based methods can capture the propagation effects inherent in hyperbolic equations and have been shown very effective in driving an hp-adaptation procedure to obtain a very accurate functional output. The objective of the present work is to extend the adjoint-based error estimate and adaptive mesh refinement algorithm for the high-order CPR method to the 3D Navier-Stokes equations. In the final paper, we will apply the proposed method to several well-known aerodynamic test cases and demonstrate its performance to 3D flow simulations.

Title: Direct Simulation of Higher-Order Stochastic Material Morphologies

Author(s): Michael Shields, Hwanpyo Kim, *Johns Hopkins U.*

Most random material morphologies possess features that cannot be captured effectively with low order moments (mean and 2-point correlation function) and the resulting properties (e.g. yield stress, permeability, conductivity) are strongly dependent on these higher-order features. Numerous efforts have been undertaken to generate artificial material morphologies possessing these stochastic features in an attempt to understand material behavior and its variability through computational simulations. The currently available methods rely on the solution of a complex stochastic inverse problem using stochastic search algorithms that are computationally expensive [Torquato,GB&Xu]. The computational expense of generating these morphologies makes Monte Carlo simulation and statistical analysis intractable. In this work, we derive the Polyspectral Representation Method, which is a broad generalization of the classical second-order Spectral Representation Method [Shin & Deo], for the direct simulation of higher-order stochastic fields. We demonstrate the general methodology through specific application of the Bispectral Representation Method (BSRM) for simulating third-order stochastic fields for material morphology simulations. The BSRM is computationally efficient and simple to implement – particularly when compared to stochastic inverse methods. Through a supporting discussion related to the estimation of polyspectra from existing data, we argue that with advancements in data collection for materials, we are entering a period where these properties can be characterized. [1] Yeong, C.L.Y. and Torquato, S. (1998). "Reconstructing random media." *Physical Review E*. 57: 495-506. [2] Graham-Brady, L. and Xu, X.F. (2008). "Stochastic morphological modeling of random multiphase materials." *Journal of Applied Mechanics*. 75: 061001. [3] Shinozuka, M. and Deodatis, G. (1991). "Simulation of stochastic processes by spectral representation." 44: 191-204.

Title: Adjoint-Based Error Estimation for Chaotic Flows

Author(s): Yukiko Shimizu, Krzysztof Fidkowski, *U. Michigan.*

Adjoint-based error estimation for mesh adaptation often outperforms other adaptation strategies for both steady and unsteady flows. However, this technique has not yet been extended to chaotic applications. This is due to the 'butterfly effect', where small perturbations in the initial condition quickly magnify and fundamentally change the unsteady trajectory, making prediction of the system after a short period of time difficult. One example of a simple chaotic system is the Lorenz attractor, a hyperbolic strange attractor that has at least one positive and one zero Lyapunov exponent. It is the positive Lyapunov exponent that causes exponential growth of initial condition perturbations. Due to the fundamental irrelevance of the initial condition for these types of problems, outputs of interest are statistics obtained over long time spans. When applying traditional unsteady adjoint techniques, even for such averaged quantities, the adjoint solution diverges backwards in time, making it impossible to perform mesh adaptation for chaotic flow. This presentation proposes a way to modify the adjoint method to accommodate chaotic flows by taking advantage of the assumption of ergodicity, which states that long term average of interested outputs of the system are independent of the initial conditions. The work is based on the least squares shadowing method [1], which given ergodicity, searches all trajectories by looking at different initial conditions until a trajectory that exists very closely to the original trajectory is discovered. Overall, the problem changes from an ill-posed to a well-posed problem. This idea of ergodicity changes the chaotic problem into an optimization problem where the distance between the two trajectories is minimized. The trajectory that is closest to the original trajectory is called the shadow trajectory. Once this trajectory is found, adjoint calculations become meaningful and useful. By combining this technique with known adjoint techniques, error estimation or mesh adaptation becomes feasible. We present results from this modified adjoint-error estimation for the Lorenz attractor and a cylinder in high Reynolds number flow, where the governing equations are solved using a discontinuous Galerkin finite element discretization in both space and time. [1] Blonigan, P., Gomez, S., and Wang, Q., "Least Squares Shadowing for Sensitivity Analysis of Turbulent Fluid Flows," 52nd Aerospace Sciences Meeting, AIAA, National Harbor, MD, 2014, pp. 1-24.

Title: Multi-Scale Simulation of Polymer Nanocomposites: Elastoplastic Approach

Author(s): Maenghyo Cho, Hyunseong Shin, Junghyun Ryu, *Seoul Nat'l. U.*

In this study, a multiscale approach to investigate plastic deformation mechanism of neat polymer and polymer nanocomposites is proposed. Many molecular dynamics (MD) studies have been carried out to characterize plastic deformation mechanism of thermoplastic polymer such as polyethylene and polypropylene. However, plastic mechanism of polymer nanocomposites structures has not been established through MD simulation yet. Moreover, reinforced filler-size dependency mechanical behavior is critical issue in mechanical design. However, for plastic materials, the interfacial behavior for various filler size has not been characterized yet. Therefore, an efficient and rigorous multiscale framework including plastic deformation mechanism has to be constructed, which is the motivation of this study. The main contributions of this study are identification of plastic deformable mechanism including damage and construction of multiscale finite element model reflecting interfacial characteristics. At the proposed multiscale model, the interface effect is reflected in the isotropic and homogenous interphase zone. Molecular dynamics simulation and a continuum nonlinear two-scale homogenization method are merged into the proposed multiscale modeling. The characterization of the condensed interphase zone between silica nanoparticle and Nylon6 polymer matrix are conducted. Nonlinear mechanical behavior of polymer nanocomposites was identified by MD simulation. Multiaxial tension/compression simulations are employed through NVT ensemble simulation including unloading simulations. The obtained stress-strain relationship of Nylon6 is fitted by elastoplastic model in this study. The elastoplastic behavior of effective interphase is quantified by iterative inverse algorithm based on the nonlinear two-scale homogenization method.

Title: Characterization of Macroscopic Strength Degradation in Polycrystalline Metals Due to Fatigue Aging

Author(s): Yuichi Shintaku, Mayu Muramatus, Shinsuke Takase, Shuji Moriguchi, Kenjiro Terada, *Tohoku U.*; Seiichiro Tsutsumi, *Osaka U.*.

We propose a two-scale analysis method to assess macroscopic strength from polycrystalline aggregates after fatigue degradation. The method hinges on numerical strength experiments (NSEs) on a representative volume element (RVE) to characterize the macroscopic mechanical behavior induced by micro-scale cracking under cyclic loading conditions. In a series of NSEs, finite element (FE) simulations are carried out with a variety of assumed macroscopic stress states to generate microscopic cracks inside the crystal grains and propagate to reduce the macroscopic strength decreases over time. To simulate the fracture behavior in the RVE, we employ a cohesive zone model (CZM) with a damage variable, which represents certain defects accompanied by ductile and fatigue fractures, within the framework of crystal plasticity and thermodynamics. Here, the damage variable is supposed to evolve with accumulated crystallographic slip deformations reflecting the reduction of the material's cohesive resistance on the generated cracks. Microscopic simulations of arbitrary crack nucleation in the RVE are realized by the embedded cohesive zone model (ECZM), which is similar to the existing rotating crack model, whereas the discontinuous displacements during the crack propagations are explicitly represented with the help of the finite cover method (FCM), which is one of the generalized finite element methods. This proposed setting for the NSEs with the CZM with ECZM enables us to evaluate the crack growth rate at micro-scale with relatively small number of cyclic loading without any other modifications like the trapezoid cohesive law for ductile fracture and the hysteretic law for fatigue fracture. We then propose a scale-up procedure of the microscopic crack growth rate to the corresponding macroscopic one, which at the same time provides the macroscopic CZM to relate the macroscopic cohesive traction and crack opening displacement. The derived macroscopic crack growth rate along with the macroscopic CZM makes the propagating crack longer than that of the microscopic one, since the damage evolution at the macroscopic primal crack surface is accelerated by the accumulation of plastic deformation with the same number of loading cycles as in the NSEs. Thus, the macroscopic strength caused by the macroscopic fatigue degradations can eventually be assessed with relatively low computational costs. Several numerical examples are presented to demonstrate such a capability of the proposed method.

Title: Numerical Simulation of Liquid-Vapor Flows with Navier-Stokes-Korteweg Equations

Author(s): Mahnaz Shokrpour Roudbari, E. Harald van Brummelen, *Eindhoven U. Tech.*; Herman M.A. Wijshoff, *Oc'e Technologies*.

Although sharp-interface models are used as conceptually straightforward methods for tracking the interface in moving boundary problems, they often lead to difficulties in resolution of the various flow singularities including topological/stress singularities in complex morphological flow transitions. Diffuse-interface models (DIM), however, provide a better alternative since they allow the computation of the fluid flow of two phases and, consequently, movement and deformation of the interface on fixed grids. This is due to the basic concept of DIM that replaces the sharp interface with a transition layer where the two phases mix to a certain degree. This study is devoted to the numerical simulation of the Navier-Stokes-Korteweg (NSK) equations known as the most accepted mathematical (phase-field) model for isothermal phase transfer problems like cavitation, bubble rising, etc.. We develop a numerical formulation based on isogeometric analysis for efficient treatment of higher-order partial-differential operators. Finally we will develop the model for the coupled Cahn-Hilliard-Navier-Stokes-Korteweg.

Title: A Parallel Framework for Multiobjective Mesh Optimization

Author(s): Suzanne Shontz, *U. Kansas.*

Parallel finite element simulations are now commonplace; such simulations are being conducted on applications in image-guided neurosurgery, incompressible fluid flow, and rockets, among others. Traditional finite element simulations require the use of high-quality, untangled meshes in order to obtain accurate analyses. In order to address this need, we propose a parallel multiobjective mesh optimization framework for mesh quality improvement and untangling for use on distributed memory machines. Our parallel framework builds upon the earlier work of Kim, Panitanarak, and Shontz as described in [1]. Algorithms within our framework are able to simultaneously optimize various aspects of the mesh, such as the element shape, element size, PDE interpolation error, and the number of inverted elements, in parallel; however, other types of improvement are also possible. We employ an edge coloring-based algorithm as in [2] for synchronizing unstructured communication among the processes while executing an algorithm within our framework. We examine the strong scaling efficiency and the weak scaling efficiency of a few algorithms within our framework as applied to simultaneous optimization of very large-scale meshes. References: [1] J. Kim, T. Panitanarak, and S.M. Shontz, "A multiobjective mesh optimization framework for mesh quality improvement and mesh untangling", *International Journal of Numerical Methods in Engineering*, 94(1):20-42, April 2013. [2] S.P. Sastry and S.M. Shontz, "A parallel log-barrier method for mesh quality improvement and untangling", *Invited submission to Engineering with Computers*, 30(4):503-515, October 2014.

Title: A Molecular Dynamics Study of the Role of Microstructure on the FCC to BCC Phase Transformation During Shock of Nanocrystalline Copper

Author(s): Mehrdad Sichani, Douglas Spearot, *U. Arkansas.*

The molecular dynamics method is used to investigate the role of microstructure on the Hugoniot state [1] and the FCC to BCC phase transformation [2] during shock of nanocrystalline copper. Particle velocities from 1.0 to 3.4 km/s are applied to a nanocrystalline copper sample with grain sizes from 6 to 26 nm. Results show that the grain size does not significantly influence the temperature and the pressure of the Hugoniot state. A FCC to BCC phase transformation is observed for pressures between 100 to 200 GPa behind the shock front and depends on grain size, grain orientation, and particle velocity. By increasing the grain size, the atomic percentage of the BCC phase increases due to the lower fraction of atoms that are positioned at grain boundaries in the original FCC nanocrystalline sample. In addition, among the particle velocities studied, the FCC to BCC phase transformation is negligible for particle velocities below 2.0 km/s, it reaches a maximum at 2.4 km/s, and then decreases from 2.4 to 3.2 km/s due to the initiation of partial melting of the nanocrystalline sample. Moreover, the FCC to BCC phase transformation strongly depends on the grain orientation. The phase transformation occurs predominantly for grains with $\langle 100 \rangle$ lattice vectors aligned with the shock loading direction, indicating that the tetragonal phase transformation path (Bain path) [3] is the mechanism by which the phase transformation occurs. [1] A. M. He, S. Q. Duan, J. L. Shao, P. Wang, and S. N. Luo, "Local and bulk melting of shocked columnar nanocrystalline Cu: Dynamics, anisotropy, premelting, superheating, supercooling, and re-crystallization.," J. Chem. Phys., vol. 139, no. 7, p. 074502, Aug. 2013. [2] A. V. Bolesta and V. M. Fomin, "Phase transition behind a shock front in polycrystalline copper," Dokl. Phys., vol. 59, no. 6, pp. 249–253, Jul. 2014. [3] L. Wang and M. Šob, "Structural stability of higher-energy phases and its relation to the atomic configurations of extended defects: The example of Cu," Phys. Rev. B, vol. 60, no. 2, pp. 844–850, Jul. 1999.

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Title: Linear Solver Strategy for Coupled and Implicit Discontinuous Galerkin Method to Model Miscible Displacement with Adverse Mobility Ratio

Author(s): Christopher Siefert, Raymond Tuminaro, *Sandia Nat'l. Lab.*; Gauthier Becker, Huafei Sun, Jichao Yin, Hao Huang, *ExxonMobil*.

A fully coupled and implicit discontinuous Galerkin formulation has demonstrated excellent accuracy and stability for the modeling of viscous fingering phenomenon occurring in miscible displacement with adverse mobility ratio. In this talk, we present a linear solver strategy which can offer this method significant speed up. Our strategy preconditions a Krylov method using block relaxation on the entire problem, coupled with a multigrid method on the pressure unknowns only. The multigrid method first coarsens in polynomial degree and then spatially. Numerical results show that the preconditioner maintains good performance over the whole fingering process. Enabled by the new linear solver, high resolution viscous fingering results in both 2D and 3D will be presented.

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Title: Simulation of Fractographic Features in Glass with Multi-Scale Peridynamics

Author(s): Stewart Silling, *Sandia Nat'l. Lab.*; Florin Bobaru, Yenan Wang, *U. Nebraska - Lincoln*.

Peridynamics is an extension of the classical theory of solid mechanics that is oriented toward problems with evolving discontinuities, especially growing cracks. Its primary advantage in modeling brittle fracture is that nucleation and growth of cracks arise spontaneously from the evolution of the dynamic field equations and material model, without the need for a supplemental mathematical relation that governs crack growth. This aspect of peridynamics may offer the potential to treat certain subtleties and instabilities in dynamic fracture of brittle materials that might be more difficult to reproduce with more standard analysis methods. The features that appear on the surface of a crack in glass, such as the mirror-mist-hackle pattern, are used by fractographers in determining the origin of structural failures and the stress conditions that the crack experiences as it propagates [1]. Many of these features arise from instabilities such as microbranches that occur as the cracks accelerate and approach their terminal velocity. The close connection of fractographic features with instability makes them an interesting problem to study with peridynamic numerical techniques. The disparate length scales of some fractographic features in glass, which can range from sub-micron initial defect to component scale fracture patterns, makes this a challenging problem that requires a multiscale technique. This talk will report on efforts to apply a recently developed concurrent hierarchical multiscale peridynamic code [2] to the problem. Applications to be discussed include failure of a glass rod from a defect under varying loading conditions. Hertzian cracking due to indentation will also be discussed. [1] G. D. Quinn, "Fractography of ceramics and glasses," US Department of Commerce, Technology Administration, National Institute of Standards and Technology (2007). [2] S. A. Silling and J. V. Cox, "Hierarchical Multiscale Method Development for Peridynamics," Sandia National Laboratories technical report SAND2014-18565 (2014)

Title: Maximizing Phononic Band Gaps in Piezocomposite Materials By Means of Topology Optimization

Author(s): Sandro Vatanabe, Emilio Silva, *U. Sao Paulo*; Glaucio Paulino, *Georgia Inst. Tech.*.

Phononic crystals (PCs) can exhibit phononic band gaps within which sound and vibrations at certain frequencies do not propagate. In these materials, large band gaps are of great interest for many applications, such as transducers, elastic/acoustic filters, noise control, and vibration shields. Previous work in the literature concentrated on PCs made of elastic isotropic materials; however, band gaps can be enlarged by using non-isotropic materials, such as piezoelectric materials. Because the main property of PCs is the presence of band gaps, a feasible alternative to design microstructures that have a desired band gap is by means of topology optimization. Thus in this work, our main objective is to maximize the width of absolute elastic wave band gaps in piezocomposite materials designed by means of topology optimization. For band gap calculation, the finite element analysis is employed together with Bloch–Floquet theory to solve the dynamic behavior of two-dimensional piezocomposite unit cells. In the topology optimization formulation, a material model based on density method is defined to interpolate two types of materials (piezoelectric and non-piezoelectric) over radiative surfaces of domain. The method of moving asymptotes (MMA) is applied as the optimization algorithm. Higher order frequency branches are also investigated. The results demonstrate that tunable phononic band gaps in piezocomposite materials can be designed by means of the present methodology and approach.

Title: Stabilizing the Orthogonal Residual Iterative Procedure with the Normal Flow Technique:
Applications to Stability of Arches

Author(s): Ricardo Silveira, Andréa Silva, *Federal U. Ouro Preto*; Dalilah Pires, *Federal U. São João Del Rei*; Gilney Gonçalves, .

An efficient nonlinear solution strategy must be able to trace the entire structural equilibrium path (or load-displacement curve), identifying and passing through the singular or critical points that may exist. A large number of the solution procedures are based on the Newton-Raphson iterative scheme (full or modified) to which are coupled the path-following methods [1]. This work uses the Newton-Raphson iteration scheme and the orthogonal residual procedure proposed by Krenk [2]. In the orthogonal residual strategy, the load parameter is adjusted using the orthogonality condition between the unbalanced force vector and the current incremental displacement vector. However, depending on the structural system analyzed, this strategy presents numerical problems or inconsistencies in nearby load or displacement limit points (snap buckling phenomena). Therefore, this work aims to present an efficient numerical procedure to stabilize the orthogonal residual strategy. It is proposed that a perpendicularity condition, referred to as normal flow technique [3], be fulfilled through the iterative solution process, so that the difficulty in overcoming all critical points along the nonlinear equilibrium path be surpassed. The numerical methodology idealized is described in detail and, to prove its efficiency, structures showing highly geometric nonlinear behavior, bifurcation points, and inelastic behavior are studied. REFERENCES [1] A.R.D. Silva, Computational system for advanced static and dynamic analysis of steel structures, PhD Thesis, Graduate Program in Civil Engineering, Deciv/EM/UFOP, Ouro Preto/MG, Brazil, (2009) (In Portuguese). [2] S. Krenk, "An orthogonal residual procedure for non-linear finite element equations", *Int. J. Num. Meth. Engng*, 38, 823-839 (1995). [3] R. Tabatabaei, H. Saffari and M.J. Fadaee, "Application of normal flow algorithm in modal adaptive pushover analysis", *Journal of Constructional Steel Research*, 65, 89-96 (2009).

Title: A Generalized Finite-Element Method Approach to Rigid Line Inclusions

Author(s): Mohsen Goudarzi, Angelo Simone, *Delft U. Tech.*.

Rigid line inclusions, stiffeners, or anticracks are some of the names that have been given to thin hard-phase inclusions. Since the pioneering work of Atkinson [1], they have been under major mathematical considerations, mainly focused on the definition of the stress state around the tip and the extent of the stress intensity factor field in homogeneous and bimaterial cases. One important feature of these inclusions is the singularity of stress components at the tip. Rigid-line inclusions (RLIs) are of importance in reinforced composite structures. For those cases with stiff reinforcements as carbon nanotubes, a rigid fiber behavior is physically realistic. This rigid behavior can lead to the formation of shear bands whose characterization can be achieved with existing analytical approaches only in simple cases. The analysis of composites with realistic RLI distributions requires accurate and robust numerical approaches. This study aims to assess the mechanical behavior of composites with RLIs using a numerical framework similar to that proposed by Radtke et al. [1]. This framework is based on the partition of unity finite element method and allows to describe RLIs by simply superimposing them on a background mesh, with no need for the background mesh to be aligned with the inclusion boundaries. Compared to the approach by Radtke et al. [1], RLIs can be thought of as fibers with high stiffness. This contribution presents a detailed study of the effective properties of RLI composites. Special attention will be paid to accurately describe the behavior of RLIs in the tip region. References [1] C. Atkinson, Some ribbon-like inclusion problems. *Int. J. Eng. Sci.* 11:243–266, 1973. [2] F. K. F. Radtke, A. Simone and L. J. Sluys, A partition of unity finite element method for simulating non-linear debonding and matrix failure in thin fibre composites. *Int. J. Numer. Meth. Eng.* 86:453–476, 2011.

Title: Hybrid KMC and Continuum Modeling of Surface Reconstruction in Silicon Nanobeams

Author(s): Amit Singh, Ellad Tadmor, *U. Minnesota.*

Silicon (001) surfaces in non-equilibrium molecular dynamics (NEMD) simulations undergo a reconstruction from the ideal diamond crystalline surface to $p(2 \times 1)$ above 20 K. The reconstruction involves the formation of rows of dimers along the $[-110]$ direction. This process results in latent heat release that causes a dramatic increase in beam temperature. We propose a hybrid continuum partial differential equation (PDE) and kinetic Monte Carlo (KMC) method to model this behavior in silicon nanobeams. An input to the method is the energy barrier for dimerization, which is computed separately using nudged elastic band calculations. The time-dependent temperature profiles along the beam predicted by the PDE-KMC method are in good agreement with results from NEMD simulations.

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

Title: Domain Decomposition and Multi-Scale Preconditioners for Heterogeneous Media Using Optimal Local Basis Functions

Author(s): Robert Lipton, Paul Sinz, *Louisiana State U.*

In this presentation we describe a new class of multiscale preconditioners using the recently developed optimal local approximation spaces developed for GFEM [1,2]. The domain decomposition employs overlapping domains within the Partition of Unity Method. We provide explicit theoretical convergence rates for the iterative method. References. [1]. Babuska, I. and Lipton, R. "Optimal local approximation spaces for generalized finite element methods with application to multiscale problems," Multiscale Modeling and Simulation, SIAM 9 2011, pp. 373–406. [2.] Babuska, I., Huang, X., and Lipton, R., "Machine computation using the exponentially convergent multiscale spectral generalized finite element method," ESAIM: Mathematical Modeling and Numerical Analysis 48 2014, pp. 493-515.

Title: Stability Analysis of Mesh-Free Methods for Landslide Simulations

Author(s): Thanakorn Siriaksorn, Sheng-Wei Chi, *U. Illinois, Chicago.*

A meshfree method based on the Reproducing Kernel Particle Method [1] is introduced for landslide simulations, which typically demand an effective numerical formulation to handle extremely large deformations and to capture both fluid-like and solid-like mechanical behaviors of soil materials. A frictional kernel contact algorithm that utilizes the interaction of kernel supports between different contacting bodies to represent contact conditions [1] is employed for dealing with interactions between damaged soil materials. Multi-field meshfree formulations are implemented in consideration of porous constitutive models, such as the Barcelona Basic Model [2] and those based on generalized Biot theory. A Drucker-Prager plasticity with damage model is also incorporated into the formulations to consider material hardening, softening, and ultimately damaged. Stabilized nodal domain integration schemes based on the framework of variationally consistent integration [3] are developed for multi-field Galerkin formulations. Several benchmark problems will be presented to verify and demonstrate the effectiveness of the proposed method. In addition, the effect of different domain integration methods as well as temporal discretization schemes on the stability of the formulations will be discussed. References [1] Chi, S.W., Lee, C.H., Chen, J.S., and Guan, P.C., "A level set enhanced natural kernel contact algorithm for impact and penetration modeling," *International Journal for Numerical Methods in Engineering*, in press, DOI: 10.1002/nme.4728 [2] E. E. Alonso, A. Gens, and A. Josa, "A constitutive model for partially saturated soils," *Géotechnique*, vol. 40, no. 3, pp. 405–430, 1990. [3] Chen, J.S., M. Hillman, and M. Ruter, "An arbitrary order variationally consistent integration for Galerkin meshfree methods". *International Journal for Numerical Methods in Engineering*, 2013. 95(5): p. 387-418.

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

Title: Predicting Mechanics of Polymeric Materials from Molecular Dynamics Simulation

Author(s): Timothy Sirk, Robert Elder, Jan Andzelm, *US Army Rsch. Lab.*

Continuum mechanical properties provide a critical bridge between the worlds of molecular simulation and experiments. However, drawing direct comparisons between the mechanical properties obtained from atomistic molecular dynamics simulation and experiments is often difficult due to vast differences in time- and length-scales, where mechanical tests in simulations are typically confined to small defect-free samples at high strain rates. The mechanics of glass-forming polymeric materials are particularly sensitive to changes in timescale, such as accelerated strain rates and cooling rates; a wide range of stress responses are possible depending on the mechanical loading conditions, thermodynamic state, the material's history, and details of the chemical composition. In this presentation, we discuss the calculation of polymeric properties using equilibrium and non-equilibrium methods and address current challenges in polymer simulation. **DISCLAIMER:** The research reported in this document was performed in connection with contract/instrument W911QX-14-C-0016 with the U.S. Army Research Laboratory. Citation of manufacturer's or trade names does not constitute an official endorsement or approval of the use thereof. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation hereon.

Title: Uncertainty Quantification of Statistical Properties of Surface Micro-Topography Using Bayesian Calibration

Author(s): Bhargava Sista, ANSYS; Sandeep Madireddy, Kumar Vemaganti, *U. Cincinnati*.

The accurate estimation of surface statistical parameters is critical to developing reliable multiscale friction models. Due to the inherent random nature of most surfaces, statistical properties calculated at different cross-sections vary from each other, which introduces uncertainty into these properties. The objectives of this study are to develop a methodology for estimating the statistical properties of surface micro-topography, to quantify the uncertainty in these parameters, and to quantify the effect of these uncertainties on the estimated spectral moments of the surface. This is achieved by calculating the numerical autocorrelation of surface heights for various cross-sections of the surface. The ensemble of these autocorrelations is represented in the form of a probability distribution function called the likelihood function. The likelihood function compares the numerical autocorrelation against an analytical autocorrelation function (ACF) and represents the probability that a given analytical ACF predicts the numerical autocorrelation. The uncertainty in the estimated ACF parameters is calculated using Bayesian calibration. The Bayesian framework combines prior knowledge of the model parameters and the likelihood of the model to calculate the posterior probability of the model parameters. As a result, we obtain a joint probability distribution of the ACF parameters instead of their deterministic estimates or marginal distributions. Our results show that there is a strong correlation between the estimated ACF parameters. This means the parameters are not independent of each other and sampling from individual marginal distributions results in biased estimates of spectral moments. Also, we show that the uncertainty in the estimated spectral moments increases with decreasing resolution.

Title: Design of Airfoils with Desired Pitching Moment Characteristics

Author(s): Jawahar Sivabharathy, Sanjay Mittal, *Indian Inst. Tech.*

Abstract Airfoils with desired pitching moment C_m and their derivative $C_{m\alpha}$ are designed for $\alpha = 4$ degree and $Re \leq 1000$. A gradient based optimization procedure based on continuous adjoint approach is formulated and implemented. The flow and adjoint equations are solved via the stabilized Finite element method. The stabilization technique used is the streamline-upwind Petrov/Galerkin (SUPG) and pressure-stabilized Petrov/Galerkin (PSPG) method. The L-BFGS gradient based optimizer is used for finding the optimal shape. The airfoil surface is parameterized using B-spline with 13 control points. The initial shape considered is the NACA 0012 airfoil. The optimized shape is found to have better stability characteristics but have lower lift and higher drag than the NACA 0012 airfoil. References [1] 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. [2] Srinath D., Mittal S., 2010. An adjoint method for shape optimization in unsteady viscous flows, *Journal of Computational Physics*, 229, 1994-2008. [3] Jameson A., 1988. Aerodynamic Design via Control Theory, *Journal of Scientific Computing*, Vol 3, No. 3, 233-260.

Title: Cloud Resolving Large Eddy Simulation of Tropical Convection

Author(s): Eric Skyllingstad, Simon de Szoeke, *Oregon State U.*

Cloud-resolving large-eddy simulations (LES) coupled to a thermodynamic ocean mixed layer are used to study the effect of large scale moisture convergence M on the convective population and heat and moisture budgets of the tropical atmosphere. Experiments are conducted for a limited area domain of ~ 500 km scale with imposed moisture convergence, M , with uniform sea-surface temperature (SST) and for a larger domain and for a larger domain without external moisture flux, but containing an imposed "warm pool" SST structure. Three simulations with M representative of the suppressed, transitional, and active phases of convection are first presented. For a limited area model without an imposed vertical velocity, M controls the overall vertical temperature structure. Moisture convergence equivalent to $\sim 200 \text{ W m}^{-2}$ (9 mm day^{-1}) maintains the observed temperature profile above 5 km denoting a balance between convective heating and radiative cooling to space. Increased convective heating for simulations with higher M is partially offset by greater infrared cooling, suggesting a potential negative feedback that helps maintain the weak temperature gradient conditions observed in the tropics. Surface evaporation decreases as large-scale moisture convergence increases, and is only a minor component of the overall water budget for convective conditions representing the active phase of the MJO. Cold pools generated by evaporation of precipitation under convective conditions are turbulent, with roughly double the wind stress of their surroundings. In the second set of experiments, the model SST is initialized with a warm patch across the center 1/3 of the domain having temperatures 3 degrees warmer than the remainder of the domain to see if SST variability can generate enough moisture convergence to counteract radiative heat loss to space. A background wind of 12 m s^{-1} is imposed aligned with the SST gradient so to minimize advection across the SST front. Simulated convection in this case is concentrated over the warm SST region and generates strong fluxes through intense surface cold pools. The combination of enhanced surface fluxes, vertical latent heat release and sinking motion in the surrounding cooler SST regions generates a vertical temperature structure that does not vary over time, similar the observed weak temperature gradient in the tropics. Preliminary analysis of the heat transport suggests that much of the warming over the cool regions results from lateral eddy heat flux convergence generated by convectively forced internal waves that propagate from the warm SST region.

Title: Fully Localized a Posteriori Error Estimation for Port Reduced Static Condensation Procedures

Author(s): Kathrin Smetana, Anthony T Patera, *MIT*.

In this talk we introduce optimal local approximation spaces for static condensation procedures and a rigorous a posteriori error bound based on local error indicators. We consider the port-reduced static condensation reduced basis element (PR-SCRBE) method [D Knezevic, DBP Huynh, AT Patera 2013], which has been developed for the simulation of large component based applications such as bridges. In an offline computational stage we construct a library of interoperable parametrized reference components; in the subsequent online stage we instantiate and connect the components at the interfaces/ports to form a system of components. To compute a finite element approximation on the component based system we use a domain decomposition approach. For an efficient simulation we employ two different types of model reduction --- a reduced basis (RB) approximation within the interior of the component and port reduction on the ports where the components connect. To construct optimal port spaces we consider component pairs and a (parameter dependent) transfer operator that maps the trace of the harmonic extensions on the boundary ports of the two-component system to the trace on the shared port. The (parameter dependent) port space is then spanned by the traces of the harmonic functions that maximize the $H^{1/2}$ -inner product on the shared port. Optimality can be inferred from the compactness of the transfer operator. For a related work in the multiscale context we refer to [I Babuska, R Lipton 2011]. We introduce a spectral greedy algorithm to construct a parameter independent port space. Within the a posteriori error estimator we assess the quality of the port reduction by using conservative fluxes [K Smetana 2015]. We adapt the standard estimators from RB methods to the SCRBE setting to derive an a posteriori error bound for the RB-error contribution. In order to combine the a posteriori estimators for both error contributions we use techniques from multi-scale methods. The error estimator is based on local component-wise element indicators and may hence be employed within an adaptive PR-SCRBE scheme. We also derive upper bounds for the effectivities both of the error estimator and the local indicators. We provide several numerical experiments that demonstrate an exponential convergence of the port reduction procedure and show that the derived a posteriori error estimator provides a sharp and effective bound of the energy error between the PR-SCRBE approximation and the reference finite element solution.

Title: A Computational Model of Tendon Remodeling

Author(s): David Smith, *U. Western Australia.*

It known that musculotendon units (for example, the triceps-surae muscle and Achilles tendon) adapt to provide economical locomotion, but there is limited understanding of how a tendon adapts to the muscle to improve muscle efficiency. There is currently no physiologically-based computational model explaining how tendon adaption occurs. Based on known information about tendon damage (for example, mechanical fatigue and proteolysis) and known information about tendon repair (for example, the synthesis of new collagen mers and subsequent polymerization), we propose processes taking place within the tendon that enables tendon remodelling. We implement this in a computational model for the (human) Achilles-soleus musculotendon unit. We show how remodelling can lead to stable and unstable states, and explain how the tendon can adapt to the muscle to improve musculotendon unit efficiency.

Title: Unstructured Mesh Partitioning for Adaptive Workflows

Author(s): Cameron Smith, Mark Shephard, *RPI*; Michel Rasquin, *U. Colorado, Boulder*; Dan Ibanez, *RPI*

Efficient parallel adaptive unstructured mesh-based workflows running on leadership class parallel systems require dynamic load balancing methods that address the balance requirements of specific workflow stages. For example, the unstructured mesh partition used by a PDE analysis driving error-based mesh adaptation can be predictively balanced prior to mesh adaptation to ensure that available memory is not exhausted and that the post adaptation balance is suitable for the analysis that follows. The analysis partition can be subsequently improved to decrease imbalances in mesh elements and the entity orders (vertices, edges, faces, regions) that are degree of freedom holders for increased scalability. Methods addressing workflow stage requirements that combine graph- and geometric-based procedures with those directly operating on the unstructured mesh will be discussed. Direct methods include a multi-criteria diffusive procedure driven by local and global topological metrics that quickly reduces load imbalances while preserving, or improving, the partition shape [1,2,3]. Partitions with imbalances exceeding 100%, as observed during predictive load balancing for mesh adaptation, are supported by merge-split improvement, MSI. MSI first creates empty parts by selecting combinations of lightly loaded adjacent parts to merge, and then splitting the heaviest loaded parts into the empty parts. Critical to the selection of merges is an automated procedure that evaluates possible combinations without incurring mesh element migration costs. Following the discussion of the underlying methods balancing results targetting stages increasing the partition size, adapting the mesh, and performing PDE analysis will be presented. References: [1] Smith, C.W., Rasquin, M., Ibanez, D., Jansen, K.E., Shephard, M.S., "Application Specific Mesh Partition Improvement", Submitted to SIAM Journal on Scientific Computing, 2015. [2] M. Zhou, O. Sahni, T. Xie, M.S. Shephard and K.E. Jansen, "Unstructured Mesh Partition Improvement for Implicit Finite Element at Extreme Scale", J. Supercomputing, 59(3): 1218-1228, 2012. [3] Parallel Unstructured Mesh Infrastructure (PUMI), <http://www.scorec.rpi.edu/pumi/> .

Title: Simulation and Design of Fiber Orientation in Products Produced with the FDM Additive Manufacturing Process

Author(s): Douglas Smith, Blake Heller, David Jack, *Baylor U.*

The Fused Deposition Modeling (FDM) Additive Manufacturing (AM) process makes general three-dimensional shaped objects from computer models by extruding a fine bead of polymer melt in layers onto a moving platform. One of the primary challenges for realizing FDM as a manufacturing method for engineering components is material selection since. Unfortunately, FDM polymer materials lack the stiffness and strength, both within the material and at material interfaces, that is found in other AM processes. Recently, short carbon fibers have been added to Acrylonitrile butadiene styrene (ABS) feedstock and Polylactic Acid (PLA) filament to strengthen and stiffen FDM products. This paper describes simulation and optimization methods that characterize the processing and consider the effect of adding carbon fibers to the PLA filament in the process design. We first consider the polymer melt flow and fiber orientation through a typical FDM nozzle. Polymer enters the flow domain as a solid, and exits into the free space at the nozzle exit as a molten material. The polymer melt is modeled as a generalized Newtonian fluid in Stoke's flow, and our axisymmetric finite element flow simulation includes the die swell expansion that occurs just outside the exit of the nozzle. Moments of the fiber orientation distribution function are computed along streamlines with Advani-Tucker (1987) orientation tensors using the Fast Exact Closure of Montgomery-Smith, et al., (2011) and the Folgar-Tucker (1984) isotropic diffusion model. Reverse orientation-flow coupling is ignored in this work. Our results show that the dominate shear flow in the melt prior to entering the nozzle region induces significant alignment in the flow direction, as expected. However, the contraction flow in the nozzle itself, and the expansion flow in the die swell disperses the orientation, particularly in the center of the flow. In addition, our extrusion flow simulations within and just outside the FDM nozzle are employed to optimize the shape of the nozzle passage to obtain a desired fiber orientation in the extruded polymer composite. Here we address die designs that produce orientations that are mostly random, and also those that are highly aligned. The design optimization problem to accomplish this includes an objective based on fiber alignment with constraints that impose the free surface flow condition in the die swell region and design sensitivities computed with finite difference methods. Our approach is shown to produce nozzle shapes that best process short fiber composites using the FDM process.

Title: A Block Variant of the COCG Method for Generalized Shifted Linear Systems with Multiple Right-Hand Sides

Author(s): Tomohiro Sogabe, *Aichi Prefectural U.*; Shao-Liang Zhang, *Nagoya U.*

The generalized shifted linear systems with multiple right-hand sides (RHSs) arise in the computation of Green's function for large-scale electronic structure theory that has a rich variety of applications to nanomaterials design. Since the number of the large sparse linear systems to be solved reaches up to one thousand together with dozens of right-hand sides, efficient solution of the linear systems plays a crucial role in boosting the speed of the whole computation. For solving the generalized shifted linear systems with a single right-hand side, the Generalized Shifted COCG method (GSCOCG) was proposed in [2], which falls in a class of Krylov subspace methods, and then its weighted quasi-minimal residual variant was given in [1], which theoretically includes the GSCOCG method. Therefore, if there are a plenty of parallel computation resources, one may use the GSCOCG method to solve the linear systems with multiple RHSs by regarding them as a set of linear systems with a single RHS. But in reality, such resources tend to be devoted to other computations, e.g. producing nonzero elements of the coefficient matrix at each iteration step due to memory restrictions. In this talk, in order to avoid consuming the limited resources, the GSCOCG method will be extended to solving the linear systems with multiple RHSs by using the shift-invariance property of block Krylov subspaces. A theoretical contribution and numerical efficiency will also be presented. Last but not least, the extended algorithm is suitable for parallel implementation, which may attract attention in the case where there are still enough parallel computation resources. References [1] T. Sogabe, T. Hoshi, S.-L. Zhang, and T. Fujiwara, Solution of generalized shifted linear systems with complex symmetric matrices, *J. Comput. Phys.*, 231 (2012), pp. 5669-5684. [2] H. Teng, T. Fujiwara, T. Hoshi, T. Sogabe, S.-L. Zhang, and S. Yamamoto, Efficient and accurate linear algebraic methods for large-scale electronic structure calculations with non-orthogonal atomic orbitals, *Phys. Rev. B* 83, 165103 (2011), pp. 1-12.

Title: A Hierarchical Interface-Enriched Finite Element Method for the Treatment of Problems with Complex Geometries

Author(s): Soheil Soghrati, Bowen Liang, Hossein Ahmadian, *Ohio State U.*; Jorge Barrera Cruz, *Ohio State U.* .

A hierarchical interface-enriched finite element method (HIFEM) will be introduced for the mesh-independent treatment of 2D and 3D problems with complex geometries. The proposed method provides an automated framework to capture field/gradient discontinuities associated with multiple materials interfaces that are in a close proximity or contact, while using finite element meshes that do not conform to the problem morphology. While yielding an optimal precision and convergence rate, one of the main advantages of the HIFEM is the ease of implementation and the ability to accommodate multiple materials interfaces in non-conforming elements. Furthermore, the construction of enrichment functions in this method is independent of the number and sequence of the interfaces introduced to non-conforming meshes. In this work, we will demonstrate the application of the HIFEM for simulating the thermo-mechanical response of heterogeneous and composite materials systems with intricate microstructures, including adhesives with embedded fillers and polymer matrix fiber-reinforced composites. We will also discuss the implementation of higher order elements, including Lagrangian and NURBS-enhanced elements in the HIFEM. Additionally, the HIFEM will be combined with a virtual microstructural characterization algorithm for the automated construction of the HIFEM discretized models. This algorithm can easily incorporate digital data extracted, for example, from SEM and micro-computed tomography images in the virtual microstructure to create models with highly realistic morphologies.

Title: Hexahedral Elements for the $H(\text{Curl})$ and $H(\text{Div})$ Spaces: Using Techniques from Mimetic Finite Differences to Improve Computational Efficiency and Accuracy

Author(s): Jerome Solberg, LLNL.

Elements from Nedelec's first family are widely used to approximate differential equations which naturally live in $H(\text{curl})$ or $H(\text{Div})$, such as the magnetic diffusion equation or Darcy flow. These elements have been shown to exhibit excellent performance in the case of tetrahedral and affine hexahedral meshes and are widely used, especially in their lowest-order manifestations. However, in recent years it has been discovered [1] that these elements exhibit reduced convergence properties (and in some cases may not converge at all) for meshes of non-affine hexahedra, especially in the case where the exterior element faces are not flat. Reduced integration techniques [2] and techniques derived from Mimetic Finite Differences [3] have both been proposed to "repair" such elements. A number of related techniques are presented and evaluated, with an emphasis on maintaining iterative solver performance and with an eye towards eventual use of these techniques in interface and embedded mesh methods. [1] Arnold, Douglas N., Boffie, Daniele and Bonizzoni, Francesca, "Finite element differential forms on curvilinear cubic meshes and their approximation properties", *Numer. Math.*, vol. 129, pp. 1-20 (2015). [2] Bochev, Pavel B. and Ridzal, Denis, "Rehabilitation of the Lowest-Order Raviart-Thomas Element on Quadrilateral Grids", *SIAM J. Numer. Anal.*, vol. 47, no. 1, pp. 487-507 (2008). [3] Wheeler, Mary, Guangri, Xue, and Yotov, Ivan, "A multipoint flux mixed finite element method on distorted quadrilaterals and hexahedra", *Numer. Math.*, vol. 121, pp. 165-204 (2012).

Title: Stochastic Analysis of Non-Local Damage in Heterogeneous Quasi-Brittle Materials

Author(s): Mazdak Ghajari, Arash Soleiman Fallah, *Imperial College London*; Mazdak Tootkaboni, *U. Mass Dartmouth*.

More often than not, natural or synthetic heterogeneous media comprise hard inclusions of high fracture toughness embedded, in a random arrangement, in soft matrices of lower fracture energies. The present work deals with the computational study of fracture in a two-dimensional heterogeneous medium consisting of circular hard inclusions interred in a soft matrix. The fracture toughness of the inclusions are assumed to be an order of magnitude higher than that of the surrounding matrix and the inclusion-boundary. The inclusions are randomly placed in the matrix and are of random dimensions. Fracture energy of the boundary between the inclusions and the matrix is different to that of the matrix. The objectives of the study are to establish a global damage parameter for such an arrangement as well as to look into the sensitivity of this parameter to uncertainties in the spatial arrangement of the inclusions, their size and the fracture properties at matrix-inclusion interface. To predict spontaneous crack nucleation and growth i.e. micro-fracture in the matrix and boundaries within the heterogeneous medium, the nonlocal continuum mechanics model viz. bond-based peridynamics is employed where the partial differential equations of classical continuum mechanics are replaced by integro-differential equations, thereby removing the singularities associated with classical continuum mechanics based models. Representative volume element (RVE) of the heterogeneous medium is loaded in simple tension and simple shear (monotonically until complete failure) to determine the upper-bound monotonic curve. Then cyclic loading is applied and based on the amount of energy dissipated, the global damage parameter is determined at each deformation level. To measure the sensitivity of the damage parameter to the uncertainties involved a global sensitivity analysis based on decomposition of variance will be used.

Title: 3D Dynamics of the Near-Surface Layer of the Ocean: Field and Computational Experiments

Author(s): Alexander Soloviev, *Nova Southeastern U.* ; Cayla Dean, Michael McGauley, *Nova Southeastern U.*

The upper ocean turbulent boundary layer is a dynamically active zone of the ocean. Fluxes of momentum, mass, heat and kinetic energy at the air-sea interface result in a variety of turbulent and organized structures developing in the near-surface layer of the ocean (Soloviev and Lukas, 2014). These structures are inherently three-dimensional (3D) and require non-hydrostatic modeling tools. We develop an approach to numerical simulation of 3D processes in the near-surface layer of the ocean using computational fluid dynamics software ANSYS Fluent. In particular, Large Eddy Simulation Volume of Fluid (VOF) method has allowed us to model the air-sea interface down to sub-millimeter scales, including surface tension effects and sea spray (spume) generation. To date, computational experiments have involved freshwater lenses, double-diffusion effects, coherent structures (Langmuir cells, ramps), large diurnal warming events, oil spills, the aqueous viscous sublayer in the presence of short gravity capillary waves, the effect of surfactants, and the air-sea interface under tropical cyclone conditions. In this paper, we consider in detail an example of 3D evolution of freshwater lenses formed due to convective rain in the Intertropical Convergence Zone and associated coherent structures. These numerical simulations were designed to elucidate the relationship between vertical mixing and horizontal advection of salinity in freshwater lenses under various environmental conditions. Available near-surface data from field experiments (Wijesekera et al. 2005, Thorpe 2004, Soloviev et al. 2014) served as a guidance for numerical simulations. The results of this study indicate that within a certain range of wind/wave conditions, 3D dynamics of the near-surface layer of the ocean are essential and cannot be successfully reproduced with a 1D model. Soloviev, A.V. and R. Lukas, 2014: *The Near-Surface Layer of the Ocean: Structure, Dynamics, and Applications* (Second edition), Springer, NY, 552 pp. Thorpe, S.A., 2004: Langmuir Circulation. *Annual Review of Fluid Mechanics* 36, 55-79. Wijesekera, H.W., C. A. Paulson, and E.D. Skillingstad, 2004: Scaled temperature spectrum in the unstable oceanic surface layer. *Journal of Geophysical Research* 109, C03015, doi:10.1029/2003JC002066.

Title: A Kriging-Based Finite Element Method for Shell Analysis

Author(s): Wichain Sommanawat, *Ubon Ratchathani Rajabhat U.*; Worsak Kanok-Nukulchai, *Asian Inst. Tech.*.

A Kriging based Finite Element Method (K-FEM) for the analysis of shell structures is presented. The proposed method is based on the bilinear degenerated shell element [1] and the Moving Kriging (MK) interpolation [3]. Intrinsically, a concept of the K-FEM is composed of two main parts. First, the MK interpolation is employed to construct shape function instead of traditional hat function in the standard FEM. Second, a nodal domain of influence (NDOI) associated with a node can be determined by a combination of element's nodes plus satellite nodes. The element's nodes are established from element connectivity in the context of FEM while the satellite nodes are obtained by extending of NDOI over one-layer of the surrounding elements of a node. Since the Kriging shape function possesses the Kronecker delta property, there is no special treatment is required at boundary conditions compared with that of utilizing Moving Least Square (MLS) approximation in the conventional element-free Galerkin method (EFGM)[2]. The formulation of the proposed shell element can be straightforwardly derived from the degenerated shell approach as in the standard FEM. In addition, the quadrilateral background cells and a reduced integration technique are adopted for numerical implementation. To assess the performance of the element, a standard set of benchmark problems for shell structure are chosen and tested [4, 5]. The numerical results indicate that the proposed shell element has a superior advantage beyond that of standard FEM. References [1] W. Kanok-Nukulchai, "A simple and efficient finite element for general shell analysis", *Int. J. Numer. Meth. Eng.*, Vol. 14, pp. 179-200, (1976). [2] T. Belytschko, Y. Y. Lu and L. Gu, "Element-free Galerkin methods", *Int. J. Numer. Meth. Eng.*, Vol. 37, pp. 299-256, (1994). [3] L. Gu, "Moving Kriging interpolation and element-free Galerkin method", *Int. J. Numer. Meth. Eng.*, Vol. 56, pp. 1-11, (2003). [4] P. Krysl and T. Belytschko, "Analysis of thin shells by the element-free Galerkin method", *Int. J. Sol. Struct.*, Vol. 33, pp. 3057-3080, (1996). [5] R. H. Macneal and R. L. Harder, "A proposed standard set of problems to test finite element accuracy", *Finite. Elem. Anal. Des.*, Vol. 1, pp. 3-20, (1985).

Title: The Tactics for Hypervelocity Impact Simulations with Use of Smoothed Particle Hydrodynamics Method

Author(s): Zhenfei Song, Shicao Zhao, Jianheng Zhao, *China Academy of Eng. Physics.*

The fragments resulted from target/projectile hypervelocity impact (HVI) is of wide concerns. In a Whipple shield for purpose of protecting structures from HVI, it uses a preplaced bumper with a stand-off to the rear wall to produce spreadable debris cloud, and therefore absorbs its dispersed momentum without structural failure. It poses a challenge for HVI simulations when considering that the fragmented particles to be formed is usually in micro meter, and that the rear wall is subjected to discrete impacts of these hypervelocity particles, not taking account of the complicated mechanism involved. The Smoothed Particle Hydrodynamics (SPH) is widely used owing to its advantages in describing the fragmentation process and tracing the fragmented particles efficiently due to the Lagrangian solved used. Special tactics were adopted herein to meet the challenge of size-scale changes as mentioned before during HVI. For Whipple structures, the generation of a debris cloud by bumper/projectile collision, expansion of the debris cloud, and deformation and damage of the rear wall by impaction of the debris cloud were simulated separately and were collected in sequence to address the various characteristic size-scales of concerns. Once the bumper and/or projectile have been melted by shock wave or its unloading, the ejecta are generally micrometer in size. It is usually beyond the scope of the size of the SPH particles in simulations. To overcome this shortcoming, the micro-ejecta model in combination with the discrete SPH particles was put forward on the basis of experimental results. An example in relation to Whipple ballistic tests was given where the radial expanding cracks and subsequent petal-shaped edge curl along the penetrating hole in the rear were simulated in agreement with the post-shock experimental observation. The shock compression and subsequent damage of fabric structures were also simulated with use of the SPH method. Since the impact response of fabric has strong locality due to shock loading, the computational model was built according to the textile substructure directly. Simulations have been performed for optimizing the shielding structure by means of the selections of fiber properties and fabric substructures.

Title: Optimal Topology Design Using Configurational Derivative and Enriched Isogeometric Analysis

Author(s): Tao Song, Hung-yun Lin, Ganesh Subbarayan, *Purdue U.*

In this presentation, a method for topological optimization through insertion and configuration of finite sized heterogeneities is demonstrated. The method relies on the recently derived Configurational Derivative [1] that describes the sensitivity of an arbitrary objective with respect to arbitrary design modifications of a heterogeneity inserted into a domain with moving boundary. The inserted heterogeneity may be a stiff or a soft inclusion, which in the limit corresponds to a hole. The Configurational Derivative takes special forms when the heterogeneity is subject to translation, rotation and uniform scaling. The Configurational Derivative may also be further simplified for special objectives such as compliance. In the limit of infinitesimal spherical inclusions, the Configurational Derivative is shown to be a generalization of the classical topological derivative. The computational implementation relies on an enriched isogeometric analysis (EIGA) [2] in the heterogeneous problem domain. The analysis is carried out by enriching the underlying approximation with an explicitly defined interface on which enrichment functions are isoparametrically described. Several numerical examples, including the optimal design of mechanical parts, are presented to demonstrate the methodology. Reference: [1] H.Y. Lin and G. Subbarayan, Optimal topological design through insertion and configuration of finite-sized heterogeneities, *International Journal of Solids and Structures*, 50 (2) (2013) 429-446. [2] A. Tambat, and G. Subbarayan, Isogeometric enriched field approximations, *Computer Methods in Applied Mechanics and Engineering*, 245-246 (2012) 1-21.

Title: A Semi-Analytical, Displacement-Based Formulation of Arbitrary Polyhedral Elements

Author(s): Chongmin Song, Hossein Talbei, Albert Saputra, *U. New South Wales*; Sundararajan Natarajan, *Indian Inst. Tech., Madras*; Ean Tat Ooi, *Federation U.*

Conventional finite element method relies on discretizing the computational domain into simplex elements, which could be restrictive in some instances, for example, meshing complex intricate shapes or moving boundary problems. Hence there is an increasing interest in employing arbitrary polygons/polyhedra within the finite element framework. In this contribution, a semi-analytical displacement based formulation of arbitrary polyhedron elements will be presented. The formulation is based on the 'scaled boundary finite element method'. The only limitation on the geometry of the polyhedron is that they have to be star convex. The volume integral is transformed to a surface integral over the faces of the polyhedron by employing the scaled boundary coordinate system. Discretization is only required on the faces of a polyhedron. Standard 2D finite elements or polygon elements with Wachspress shape functions can be used. The semi-analytical formulation allows efficient treatment of stress singularity problems without asymptotic enrichment. The application of the present formulation to octree meshes is also discussed, as it is an ideal choice for constructing elements with arbitrary number of nodes on a particular face occurring in an octree mesh. The convergence properties and the accuracy of the present formulation are demonstrated with a few benchmark problems from linear elasticity. Extension to higher-order polyhedron elements and applications in linear elastic fracture mechanics will also be discussed.

Title: A Localized Version of Mortar Method for Treatment of Three-Dimensional Non-Matching Interfaces

Author(s): Yeo-ul Song, Sung-Kie Youn, *KAIST*; Kwang-Chun Park, *U. Colorado*.

The proposed algorithm presents a localized version of mortar method. We construct a special interpolation treatment using the method of localized Lagrange multipliers for non-matching interfaces constraint functional in three-dimensional problems[1]. The classical mortar method for arbitrary dissimilar three-dimensional meshes was developed by Puso[2]. It requires several steps in numerical integration of the correlated master-slave elements. In the contact problems of structures, which have the curved interfaces, the classical mortar method needs additional efforts in order to satisfy the angular momentum conservation[3]. For many dynamic problems that undergo rotational motions, large numerical errors may occur along the interfaces unless the interface treatment satisfies the angular momentum conservation. The present method provides conservation of the linear and angular momentum. It is shown that the gaps in the interfaces can be handled appropriately without the spurious straining through the numerical examples [1] Park KC, Rebel, G, Felippa CA. A simple algorithm for localized construction of non-matching structural interfaces. *International Journal for Numerical Methods in Engineering* 2002; 53:2117-2142. [2] Puso, MA. A 3D mortar method for solid mechanics. *International Journal for Numerical Methods in Engineering* 2004; 59:315-336. [3] A mortar method for energy-momentum conserving schemes in frictionless dynamic contact problems. *International Journal for Numerical Methods in Engineering* 2009; 77:1468-1500

Title: Two-Scale Modeling of Progressive Failure in Partially Saturated Porous Media

Author(s): Xiaoyu Song, *U. Florida*; Joshua White, *LLNL*.

Partially saturated porous media (e.g., unsaturated sands) have a natural internal pore structure in which two fluids (e.g., water and air) coexist in the pore space. This pore structure is generally heterogeneous, which makes unsaturated porous media susceptible to progressive failures (e.g., shear banding). In the paper, we present a two-scale mathematical framework to model the mechanical and transport properties in partially saturated porous media during the localized deformation process. In this framework, the deformation of solid skeleton is described by a three-invariant elasto-plasticity constitutive law recently proposed by the authors. The salient feature of this phenomenological constitutive law is that it can characterize the heterogeneities of porosity and meniscus strength at meso-scale. The initiation of localized deformation triggered by material heterogeneities is detected if the “drained acoustic tensor” condition is satisfied. The fluid flow inside the localized zone (the micro-scale) is modeled independently from the fluid flow in the bulk porous media (the continuum scale). The propagation of the shear band is simulated by using the partition of unity property of shape functions of finite element. Numerical examples are presented to demonstrate the performance of the approach.

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Title: Fluid-Structure Interaction in Engineering, Environmental and Biological Flows

Author(s): Fotis Sotiropoulos, A. Gilmanov, A. Calderer, A. Khosronejad, *U. Minnesota.*

We have developed a versatile computational approach from simulating FSI problems in a broad range of complex flows involving arbitrarily complex rigid and deformable bodies and occurring across a range of Reynolds numbers and flow regimes. The method is based on the curvilinear immersed boundary method and incorporates loose and strong coupling FSI schemes for robust and efficient solutions even at low mass ratios. Large-eddy simulation with wall models is utilized to simulate turbulent flows while a level-set approach is employed for two-phase flow problems. In the talk, we will present several examples demonstrating the ability of the method to simulate FSI problems in: cardiovascular flows, aquatic swimming, wind and wave energy flows, and river flows over mobile sand beds.

Title: A Mixed Strain/Displacement Finite-Element Formulation Suitable for Fracture Computation in Large-Deformation Coupled CFD/CSD Blast and Impact Problems

Author(s): Orlando Soto, Joseph Baum, *Applied Simulations Inc.* ; Rainald Lohner, *George Mason U.*

Theoretical modelling and computational resolution of the strain localization process up to structural failure remained an open challenge in computational solid dynamics (CSD). To date, most attempts to model discontinuities with standard local approaches produce non-physical solutions, which are fully determined by mesh resolution and orientation. Cervera et al. (see [1]) showed this must be due to the poorly numerical approximation that is obtained if irreducible formulations are used (standard displacement formulations). The previous statement may be simply explained by taking into account that in irreducible formulations, the strain, which is the variable of most interest for fracture prediction, are obtained by differentiation of the fundamental unknowns (the displacement field). Hence, if linear (or tri-linear) FE are used, the strain field has a theoretical convergence of order $O(h)$ in L_2 -norm (h is the mesh size). Therefore, the strain field has zero point convergence order (in L_∞ -norm), which means that even though the mesh resolution is improved, point values do not converge. Since point strains and/or stresses (values at integration points) are used to predict material damage and element fracture, it is of no surprise that localization bands strongly depends on the mesh size and orientation. Contrariwise, when using the strain and displacement fields as primary variables of the formulation, the added accuracy and convergence seems to be enough to satisfactorily solve the mentioned mesh dependency problem (see [1] and references therein). Herein an explicit, strain/displacement, large-deformation FE formulation to deal with strong coupled CFD/CSD (computational fluid dynamics/computational solid dynamics) problems is presented. It is widely known that, if standard equal interpolation is used for the spatial discretization of both fields, strain and displacement, the scheme locks and produces meaningless and not stable results since the inf-sup condition is not fulfilled. However, equal continuous FE functions are highly desirable from a computational point of view. Hence, to circumvent the severe restrictions imposed by such an inf-sup condition, in this work the weak forms of the mixed strain/displacement solid dynamic equations are obtained by a variational multiscale stabilization (VMS) approach. Time discretization of the final continuous forms is achieved by an explicit Newmark scheme, and the spatial one by using Q1/Q1 and P1/P1 standard functions. Several VMS methods were developed in [1] for the small-deformation static solid equations, and successfully applied to localization problems: Totally physical and mesh independent solutions were obtained where the standard displacement formulation failed miserably. Finally, the CSD approach is loosely coupled with the widely tested CFD code FEFLO to solve real blast and impact problems (see [2]). Several benchmark cases and real applications will be presented. References [1] M. Cervera, M. Chiumenti and R. Codina, "Mixed stabilized finite element methods in nonlinear solid mechanics. Part I: Formulation", CMAME, Vol. 199, pp. 2559-2570, (2010). [2] O. Soto, J. Baum and R. Löhner, "An efficient fluid-solid coupled finite element scheme for weapon fragmentation simulations", Engr. Fracture Mech., Vol 77, 549-564 (2010).

Title: Multiscale Simulation of Observed 3D Crack Evolution in a Polycrystalline Aluminum Alloy

Author(s): Ashley Spear, Alexander Douglass, *U. Utah*; Jacob Hochhalter, *NASA*; Albert Cerrone, *GE Global Rsch.*

Improved understanding and predictions of structural-failure evolution across length scales requires combined advancements in experimental observations, high-fidelity multiscale modeling, data mining, reduced-order modeling, and uncertainty quantification. This work addresses a portion of these advancements by numerically reproducing the complex, 3D, crack-shape evolution observed in a polycrystalline aluminum alloy extracted from an aerospace component. The post-mortem measurements were collected in previous work* using a combination of scanning electron microscopy, X-ray computed tomography, and high-energy X-ray diffraction microscopy. The experimental data were combined to characterize incremental 3D crack-growth rates along with the grain morphologies and crystal orientations in the neighborhood of a dominant fatigue crack. These results revealed considerable variability in the local growth rates and crystallography of the 3D crack surface. However, the interactions of microstructure-sensitive fields (e.g. stress, slip) with the evolving crack front were not captured in the experimental data. The current work focuses on reproducing the observed crack-evolution process in a computational framework, thereby enabling interrogation of microstructure-sensitive fields in the neighborhood of the measured crack fronts. A significant portion of the work entails developing algorithms to generate high-fidelity finite-element (FE) meshes that explicitly contain the incremental crack shapes measured in the experiment. A concurrent multi-scale modeling technique is employed, wherein the FE mesh representing the cracked, polycrystalline sub-volume is directly embedded within a continuum-scale FE mesh of the global fatigue specimen. The concurrent coupling is needed since the specimen deforms non-uniformly due to its geometrical asymmetry. The polycrystalline and continuum regions are modeled using crystal plasticity and von Mises plasticity, respectively. In addition to the HPC resources needed to reconstruct the experimental data and generate the FE meshes, considerable computational effort is required to drive the simulations of crack evolution. The concurrent multi-scale FE model comprises approximately 50M degrees of freedom. Both cyclic loading and crack advance are simulated using a parallelized FE solver on ~5000 processors on NASA's Pleiades supercomputer. Future work will require HPC resources to mine the extensive FE results to help elucidate and quantify the variability in microstructure-sensitive, crack-shape evolution, providing an important step toward improving predictions of structural failure in engineering applications. * Spear, A.D., Li, S.F., Lind, J.F., Suter, R.M., Ingraffea, A.R. *Acta Materialia*. 76:413-424. 2014.

Title: Influence of Point Defects and Grain Boundaries on the Mechanical Strength of Monolayer Molybdenum Disulphide (MoS₂)

Author(s): Khanh Dang, Douglas Spearot, *U. Arkansas*.

As a two-dimensional material, monolayer MoS₂ possesses very unique and promising mechanical and electrical properties. However, the role of point and line defects on mechanical behavior has not been explored. In this work, molecular dynamics simulations using a reactive empirical bond order potential are performed (1) to gain insight into the failure mechanism of monolayer MoS₂ by modeling nanoindentation on a suspended free standing membrane, analogous to recent experiments, and (2) to explore the influence of point and line defects on the mechanical properties of monolayer MoS₂. Results show that the force required for fracture of the monolayer MoS₂ membrane increases with increasing nanoindenter diameter. This relationship and the magnitudes of the breaking forces computed in this work are consistent with experiments in the literature. A phase transformation, caused by an abrupt change in the S-S intralayer spacing, is observed prior to failure. For monolayer MoS₂ with point defects, the phase transformation initiates from clusters of neighboring point vacancies. For monolayer MoS₂ with grain boundaries, molecular dynamics simulations indicate that the fracture strength is independent of the grain boundary energy.

Title: IGA Suitable Planar Domain Parameterization with THB-Splines

Author(s): Antonella Falini, Jaka Špeh, Bert Jüttler, *Johannes Kepler U.*

Isogeometric analysis (IGA) uses spline parameterizations to describe the geometry of the physical domain. If such a parameterization is not available, it has to be generated from the domain boundaries. The construction of a good parameterization (bijective, regular at every point) is crucial since it strongly influences the accuracy of the subsequent analysis. It is of interest to use adaptive techniques such as hierarchical splines, since this facilitates an accurate representation of detailed geometries with a low number of degrees of freedom. We present three levels of domain parameterization techniques that are based on truncated hierarchical (TH) B-splines. The methods address the trade-off between computational effort and level of difficulty of a specific instance of the problem. The simpler methods work for relatively simple domains, while more complicated shapes require additional efforts. The direct linear method exploits the adaptivity in order to obtain highly accurate representation of the boundary and uses simple linear functionals to determine the inside of the parameterization. This approach is arguably the easiest to implement, but it is characterized by a regularization parameter. The direct non-linear method employs various quality measures to improve the properties of the domain parameterization. This method can solve a larger set of problems than direct linear method. Unfortunately, it also introduces new user-defined parameters. The indirect method uses the boundary element method to solve the Laplace's equation on the domain. Once the harmonic function is determined, it is employed to determine the interior of the parameterization. This method is free of user-defined parameters and there are theoretical results available that guarantee a regular result for sensible input. The downfall of the indirect method is that it is computationally more expensive than the direct ones. Finally, we present numerical examples that demonstrate the potential of each method. More precisely we will use the obtained parameterizations for isogeometric simulations.

Title: Extended Finite Element Method in Multiphysics Nuclear Fuel Simulations

Author(s): Benajmin Spencer, *Idaho Nat'l. Lab.*; Ziyu Zhang, John Dolbow, *Duke U.*

The vast majority of commercial nuclear power reactors worldwide employ fuel systems that consist of ceramic uranium oxide fuel pellets contained in a metallic cladding. Because of the brittle nature of this fuel material, it experiences significant fracturing, beginning with the first time the fresh fuel is brought to power in the reactor. This fracturing has a significant effect on the thermal and mechanical behavior, and hence, on the performance of the fuel system. To adequately capture the behavior of the fuel/cladding system, it is critical that nuclear fuel simulations capture the tight coupling between the thermal and mechanical response. The BISON fuel performance code [1] employs the capabilities of the MOOSE framework to solve this coupled system of physics equations. The extended finite element method (XFEM) has been implemented using the phantom node approach [2] in this multiphysics solution environment to enable the simulation of fracture in a discrete, mesh-independent manner. The mesh cutting algorithm of [3] has been adopted to determine the evolution of the mesh topology due to the propagating crack network, including crack coalescence and branching. This algorithm has been implemented using a straightforward scheme to characterize partial elements cut by crack planes and identify connections between partial elements. By employing the phantom node approach in this setting, when elements are cut, discontinuities are automatically introduced in all solution fields in the simulation. In a nuclear fuel simulation, discontinuities are introduced in both the temperature and displacement fields, which is essential for accurately accounting for the effects of fracture on all aspects of the solution. The effectiveness of this approach is demonstrated on simulations of fracture in ceramic nuclear fuel early in its life in the reactor. 1. R. L. Williamson, J. D. Hales, S. R. Novascone, M. R. Tonks, D. R. Gaston, C. J. Permann, D. Andrs, and R. C. Martineau. Multidimensional multiphysics simulation of nuclear fuel behavior. *J. Nuclear Materials*, 423:149– 163, 2012. 2. A. Hansbo and P. Hansbo. A finite element method for the simulation of strong and weak discontinuities in solid mechanics. *Comp. Meth. Appl. Mech. Eng.*, 193(33-35):3523–3540, 2004. 3. C. L. Richardson, J. Hegemann, E. Sifakis, J. Hellrung, and J. M. Teran. An XFEM method for modeling geometrically elaborate crack propagation in brittle materials. *Int. J. Num. Meth. Eng.*, 88(10):1042–1065, 2011.

Title: Quantifying the Impact of Numerical Errors Along with Other Uncertainties on Hazard Forecasting

Author(s): Elaine Spiller, *Marquette U.*; Hossein Aghakhani, Abani Patra, Bruce Pitman, *U. Buffalo.*

To forecast a geophysical hazard, one must combine 1) a stochastic scenario model – incorporating data and expert opinion – that describes the system's aleatory variability, and 2) a physical model, typically pde based, which lets one explore catastrophic hazards (inundation by flooding, landslides, tsunamis, etc). Geophysical modelers often assume that uncertainty \gg numerical error and ignore impacts of the later. We have devised a surrogate-based strategy using adjoint error estimates to quantify the effects numerical errors and other uncertainties on hazard probabilities.

Title: Unstructuring Methods for Pervasive Fragmentation Simulations in Three-Dimensions

Author(s): Daniel Spring, *U. Illinois, Urbana-Champaign*; Glaucio Paulino, *Georgia Inst. Tech.*.

There are few methods capable of simulating the full spectrum of pervasive fracture behavior in three-dimensions. Throughout pervasive fracture simulations, many cracks initiate, propagate, branch and coalesce simultaneously. Because of the cohesive element method's unique framework, this behavior can be captured in a regularized manner. The focus of this work is on the investigation of homogenized materials; however, we recognize that all materials contain heterogeneity (or defects) at the microscale. Defects naturally arise in materials due to grain boundaries, voids, or inclusions. As well, defects may be introduced through the act of processing or machining the material. These microscale defects constitute potential regions where stresses can concentrate and lead to damage or failure. To represent such heterogeneity, a statistical distribution of material properties is used. The behavior of brittle materials undergoing pervasive fracture and fragmentation is examined using three examples. The examples are selected to represent some of the significant influencing factors on pervasive fracture and fragmentation; including, geometric features, loading conditions, and material gradation. Through the examples, we demonstrate that fragmentation behavior can be regularized with the use of simple geometric features or the use of functionally graded materials. Additionally, throughout our investigation, we investigate and quantify the ability of three-dimensional nodal perturbation techniques to introduce geometric unstructuredness into a finite element mesh. References [1] D. W. Spring and G. H. Paulino. Numerical Unstructuring as a Means for Achieving Pervasive Fracture and Fragmentation in Three-Dimensions. Under Revision

Title: Multi-Scale, Transient Dynamic Analysis of Heterogeneous Materials Using Computational Homogenization

Author(s): Ashwin Sridhar, Varvara Kouznetsova, Marc Geers, *Eindhoven U. Tech.*

This work presents an efficient numerical multiscale method for modeling transient dynamic behavior of heterogeneous materials. Research on certain phenomena resulting from the interaction of elastic waves with constituent heterogeneities has shown the possibility of promising applications in the field of acoustics. However, the current methods available to model such materials are restricted to linear behavior without losses and in general lack the versatility to model real world engineering problems. Such limitations can be overcome by employing computational homogenization techniques in the case where the wavelength of the propagating elastic wave is much larger than the size of the heterogeneities. In this work, the classical computational homogenization technique is extended to a transient dynamic setting. An enriched kinematic description of the macro-micro coupling is applied where the microscopic displacements are coupled to the macroscopic displacement in addition to the deformation. The extended Hill Mandel condition is used to obtain the expressions for the macroscopic stress and momentum. The full balance of the linear momentum is solved at both scales. An attempt at developing a such a computational homogenization scheme suitable for modeling heterogeneous materials has already been made [1]. The same framework is adopted here but a completely different approach is used in the implementation of the coupling equations between the two scales. By coupling the macroscopic displacement to the overall rigid body displacement of the Representative Volume Element (RVE) instead of its microscopic displacements, the resulting expressions turn out to be more numerically efficient to implement. The nested transient solution schemes needed to solve the total problem are also discussed. The results obtained from the simulation are compared with Direct Numerical Simulations in order to verify the method. References [1] K. Pham, V.G. Kouznetsova, M.G.D. Geers, Transient Computational Homogenization for Heterogeneous Materials under Dynamic Excitation, *Journal of the Mechanics and Physics of Solids* 61 (2013) 2125-2146.

Title: A Robust Composite Time Integration Scheme for Snap-Through Problems

Author(s): Ilinca Stanciulescu, Yenny Chandra, Yang Zhou, *Rice U.*

The simulation of complex systems is important in many fields of science and in real-world applications. Time integration, if not designed properly, can return misleading numerical solutions (unstable numerical solutions for what is in fact a stable system or vice versa). We propose a robust time integration scheme for nonlinear dynamic analysis with particular application to snap-through buckling of shallow arches. The algorithm is a composite method that consists of three sub-steps. Our goal is to guarantee the stability properties of the simulated representation of the continuous system. We will achieve this goal by comparing the stability conditions of the discretized system with those of the continuous system to analyse algorithmic robustness. Numerical damping is introduced to the system by employing an algorithm similar to the backward differentiation formulas (BDF) method in the last substep. Optimal values of the algorithmic parameters are determined to satisfy stability criteria and minimize damping. The proposed method is accurate, numerically stable, and efficient as demonstrated through several examples involving large deformation, large displacement and large rotation presented in this talk.

Title: The Space-Time Version of The NURBS-Enhanced Finite Element Method (NEFEM) For Free-Surface Flow Computations

Author(s): Atanas Stavrev, *AICES RWTH Aachen*; Philipp Knechtges, Elgeti Stefanie, Marek Behr, *CATS RWTH Aachen*.

The accurate computation of geometric quantities like curvature and normal vectors plays a crucial role for the quality of free-surface flow simulations. Assuming standard, isoparametric linear finite elements, even for simple flow problems, an extensive mesh refinement might be necessary to capture geometric features of the domain and superfluous degrees of freedom are introduced just for geometry handling. A promising approach to overcome this problem is to improve the quality of the boundary representation. Recently, Sevilla et al. discussed such methodology called the NURBS-enhanced finite element method (NEFEM) [1], which is based on the standard finite element method, but also considers NURBS-geometry information. The application of the NEFEM to free-surface flows requires the method to allow for time integration in a space-time context and derivation of a kinematic rule for the NURBS movement in time. Thus, a space-time version of the NEFEM is introduced, following the procedure described by Tezduyar et al. in [2]. The spatial NURBS-enhanced element is extruded into the time domain. The new element utilizes the Cartesian FEM to define the interpolation functions (Lagrange polynomials) directly in the physical space and a suitable geometry mapping, which accounts for the NURBS movement in time. Furthermore, the variational formulation is written over the whole space-time domain and automatically considers arbitrary deformations. These are defined by a kinematic rule, which prescribes the boundary movement, i.e., the movement of the NURBS describing the free surface. However, kinematic rules use velocity information, which is available only for the finite element nodes and not for the NURBS control points. Consequently, a fitting algorithm is developed in order to project the fluid velocity into the NURBS space and use it for displacement of the control points. The performance of the space-time NEFEM is compared to the standard FEM on 2D and 3D free-surface examples. [1] R. Sevilla, S. Fernández-Méndez and A. Huerta: NURBS-Enhanced Finite Element Method (NEFEM), *Internat. J. Numer. Methods Engrg.* 76(1):56– 83, 2008. [2] T.E. Tezduyar, M. Behr, S. Mittal and J. Liou: A new strategy for finite element computations involving moving boundaries and interfaces - the deforming-spatial-domain/space-time procedure: II. Computation of free- surface flows, two-liquid flows, and flows with drifting cylinders, *Comp. Methods Appl. Mech. Engrg.* 94(3):353-371, 1992.

Title: Computational and Experimental Investigations of an Explosively-Driven Shock Tube

Author(s): Joel Stewart, Collin Pecora, *US Army Rsch. Lab.*

The U.S. Army Research Laboratory has recently used computational methods to design an explosively-driven conical shock tube, which was subsequently built and investigated experimentally. The experimental results compare well with computational results in demonstrating that full-scale blast effects (e.g., a 680 g spherical charge) can be approximated using a conical shock tube combined with a much smaller explosive charge (e.g., a 14.5 g shock tube driver charge). The study of air blast and its effects on personnel and structures is important to being able to design more effective protective equipment from events such as the detonation of improvised explosive devices. Explosively-driven shock tubes, while presenting safety and handling concerns, can provide more realistic approximations to free-field detonations than those provided by gas-driven shock tubes [1]. Additionally, a conical shock tube's geometry naturally approximates a sector cut from a spherically-symmetric blast, leading to better agreement with the blast profiles of free-field detonations when compared to those provided by shock tubes employing constant cross sections [2]. By constraining an explosive charge and the resulting blast wave with a high shock-impedance material, large blasts (which can add significant damage and safety constraints but are representative of full-scale munition effects) can be simulated with significantly smaller explosive charges.

1. Courtney E, Courtney A, Courtney M. Shock Tube Design for High Intensity Blast Waves for Laboratory Testing of Armor and Combat Material. *Defense Technology*. 2014;10:245-250. 2. Filler WS. Measurements of the Blast Wave in a Conical Tube. *The Physics of Fluids*. 1960;3(3):444-448.

Title: Microtubule Buckling In Platelet Morphogenesis

Author(s): Wylie Stroberg, Miguel Bessa, Wing Kam Liu, Seth Lichter, *Northwestern U.*

Blood platelets form from mature megakaryocytes in a complicated multi-stage process that remains poorly understood. During the final stages of platelet formation, platelet precursors, called preplatelets, undergo a microtubule-driven structural transformation from spherical to bar-bell shaped, before eventually separating into platelets. Initially, a band of several microtubules form at the equator of the preplatelet. Driven by the motor protein dynein, microtubules in the band slide against one another extending the contour length of the band. The preplatelet membrane cortex deforms to accommodate the growing band. Eventually, the growing microtubule band reaches one of two fates: either the force required to further deform the cortex is greater than the stall force of the dynein motors, and the growth is arrested, or the force applied to the microtubule band by the cortex is large enough to cause the circular band to buckle. In the first case, the result is a stable, discoidal platelet, whereas in the second, the buckling initiates the transformation to bar-bell shaped species and further subdivision of the preplatelet. Using variational methods, we show that the length-scale dependence of the transition from arresting to buckling behavior dictates platelet size. We verify our analytical solution, and investigate the post-buckling behavior of the extending microtubule band using multi-scale finite element simulations in which the extension of the microtubule band is informed from explicit molecular simulations of microtubule sliding driven by dynein motors. Using our calculations, we make predictions about the effects of dynein and tubulin concentration, as well as cortex rigidity on platelet size. These predictions suggest possible treatment strategies for giant platelet syndromes, as well as provide guidelines for engineering functional artificial platelets.

Title: Enriched Isogeometric Analysis for Explicit Tracking of Evolving Boundaries

Author(s): Tao Song, Kritika Upreti, Ganesh Subbarayan, *Purdue U.*

Phase boundaries, crack surfaces or singular points are, geometrically speaking, lower-dimensional features relative to two- or three-dimensional geometrical domains. Often, the distinguishing characteristics of the behavior at these features are known apriori and may be exploited to enrich isogeometric models. In this presentation, we describe a modeling strategy in which the geometry of the enriching entity is explicitly tracked. The base approximations are enriched isogeometrically with parametrically defined lower-dimensional entities and by constructing distance fields from them. A purely algebraic, and computationally efficient technique is utilized for constructing distance measures from NURBS entities that retain the geometrical exactness of the boundaries while eliminating the need for either a polytope approximation to the boundary and/or an iterative solution to determine the exact distance to the boundary. This in turn enables one to explicitly, efficiently, and accurately compute normals and curvatures at points on the interface or boundary. The enriched isogeometric analysis is demonstrated on a variety of applications: for tighter CAD/CAE integration through analysis of B-rep models without needing trivariate NURBS approximations, modeling of material damage as well as crack propagation, and to simulate solidification/melting by modeling geometrically explicit interface on which the interfacial Stefan condition and the Gibbs-Thomson condition are enforced. **KEYWORDS** Embedded boundaries; Isogeometric analysis; Algebraic distance field;

Title: Asynchronous Space-Time Algorithm for Computational Structural Dynamics

Author(s): Waad Subber, Karel Matous, *U. Notre Dame*.

The traditional domain decomposition algorithms for large-scale structural dynamics problems involve spatial partitioning of a computational domain and marching all the subdomains in time using a unified time step. The local subdomains discretization and time step size are typically dictated and controlled by a global error estimation criteria. This classical approach imposes a restriction that the smallest subdomain spatial and temporal scales govern the mesh and time resolutions of the rest of the structure. Furthermore, in practical large-scale engineering problems featuring localized phenomena, it is essential to focus computing power where needed. Thus a localized treatment of the mesh and time resolutions is required to efficiently capture the local spatial and temporal scales of such multi-scale problems. In other words, the computational subdomains should be independently refined in the spatial and temporal directions based on the local space and time multi-scale features of the problem. The local treatment of the spatial and temporal resolutions however, often leads to non-matching meshes along the interfaces and subdomains with heterogeneous time step sizes. To this end, we propose a Parallel Asynchronous Space-Time Algorithm based on the Domain Decomposition Method (PASTA-DDM) for structural dynamics problems on non-matching meshes. The algorithm is based on the dual domain decomposition approach. For accuracy and fulfilling the conservation requirements, we adopt the common refinement interface to transfer data among the adjacent subdomains with non-matching meshes and different time steps. To enforce the kinematic continuity constraints along the common interface, we utilize the localized Lagrange multipliers in the space and time directions. The proposed algorithm is easily parallelizable and well suited for heterogeneous computing environment. For linear dynamical problems, PASTA-DDM maintains second order spatial and temporal convergence properties, shows unconditionally stable behavior and ensures conservative of physical quantities along the interfaces. For the numerical application, we consider a sandwich plate impacted by a projectile. Based on the physical properties of the problem, the computational domain is split into a number of non-overlapping subdomains. The subdomain meshes and time steps are selected based on the local dynamical behavior of the multi-scale problem leading to large degree of asynchrony.

Title: Multi-Scale Simulations for Ductile Failures with Microscopic Void Growing

Author(s): Hirofumi Sugiyama, Kazumi Matsui, Takuya Endo, Shingo Inami, Takahiro Yamada,
Yokohama Nat'l. U..

This paper examined the relation between the macroscopic damage evolutions in damage mechanics and the microscopic void growing behaviors by using multi-scale simulations. Developing the mechanical properties of dual-phase steel has been still the basic interests in many fields of engineering. In nowadays, the finite element simulations play important roles to predict the mechanical behaviors of structures and a lot of material models have been proposed by many researchers to do the complex material behaviors. Especially, the ductile properties of metals are important to control the failure mode of structures and materials. The continuum damage mechanics has been developed for that purpose, and relates the microscopic voids and the macroscopic damage parameters. For example, Gurson-Tvergaard-Needleman (GTN) model and Lemaitre damage models are commonly accepted in our engineering fields to simulate the ductile behavior of metals. These assume that the microscopic voids govern the ductile failures and that their mechanisms consists of three major steps; the nucleation, the growth and the micro cracking. The so-called damage parameters (void volume fractions) are major state variables, and their evolution laws are main interests in these kinds of mathematical models. However, these phenomenological modeling approaches usually suffer from the increasing “the phenomenological parameters” to model more complex behaviors. On the other hand, multi-scale modeling schemes based on the mathematical theory of homogenization, have been introduced for studying micro-macro coupled behaviors and widely accepted by their capability to simulate the macroscopically complex responses from their microscopic simulations for unit-cells. In this paper, to understand the elementary process of the ductile failures with micro voids, the multi-scale simulation was executed for unit cell with simple microscopic voids. Here firstly focuses on the void growth process in microstructures and assume that there are some discontinuous boundaries (micro voids) in the microscopic structures. Constructing the various types of microscopic structures such as the different pattern of the initial void length or angle. Consequently, we confirm the correlation between the calculated void volume fraction and the macroscopic mechanical properties.

Title: Improving MPM

Author(s): Deborah Sulsky, Ming Gong, *U. New Mexico.*

The material-point method (MPM) was introduced about 20 years ago and is a versatile method for solving problems in continuum mechanics. The flexibility of the method is achieved by combining two discretizations of the material. One is a Lagrangian description based on representing the continuum by a set of material points that are followed throughout the calculation. The second is a background grid that is used to solve the continuum equations efficiently. There are four steps in the algorithm: (i) choose a convenient computational grid; (ii) map information from the material points to the grid; (iii) solve the field equations on the grid; and (iv) update the material points based on the grid solution. Examples in the literature showed some applications that appear to be second order accurate and other that appear less accurate, or even non convergent. This talk will provide analysis of the order of accuracy of MPM to shed light on these observations. Moreover, the analysis suggests modifications to the algorithm to achieve higher order accuracy. Each of the steps in the algorithm contributes to the overall accuracy and modifications must be made consistently to obtain a desired accuracy. The analysis also points to connections between MPM and other meshfree methods.

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Title: A Coupled Implicit and p-Adaptive Discontinuous Galerkin Method for Miscible Displacement with Adverse Mobility Ratio

Author(s): Huafei Sun, Hao Huang, Aruna Mohan, Jichao Yin, *ExxonMobil*; Gauthier Becker, *ExxonMobil* Co.; Chris Siefert, Ray Tuminaro, *Sandia Nat'l. Lab.*.

Many EOR or stimulation processes require an accurate estimation of the distribution of the injected fluid. Traditional reservoir simulators based on low-order finite volume method suffers from grid orientation effects when modeling miscible displacement with an adverse mobility ratio. In this talk, we propose a fully-coupled and implicit high-order discontinuous Galerkin (DG) formulation that can accurately compute the flux direction and effectively remove the grid orientation effects. A p-adaptive scheme is also developed for computational efficiency such that higher-order approximation is used only in elements with large numerical error estimates. A multigrid-preconditioned Krylov method is employed for the resulting linear system and achieves good performance. Enabled by the adaptation and the linear solver, viscous fingering results in two and three dimensions will be presented.

Title: CFD-DEM Simulations of Sediment Transport Based on a Novel Coarse-Graining Algorithm

Author(s): Rui Sun, Heng Xiao, *Virginia Tech.*

In this work, dense-phase sediment transport is simulated by using a CFD—DEM (computational fluid dynamics—discrete element method) solver with a novel, diffusion-based coarse-graining algorithm recently proposed by the authors. The present simulations employ turbulence-resolving LES (large eddy simulation) for fluid flow and utilize DEM to resolve the motions of and the collisions among individual sediment particles. The coarse-graining algorithm is used to obtain the solid volume fraction, particle phase velocity, and fluid-particle interaction forces in the fluid-particle coupling. Since the diffusion-based coarse graining algorithm has been demonstrated to be mesh-independent [1-2], the sizes of CFD cells can be either larger or smaller than the size of the particles, determined purely based on the requirements from the LES and not by the particle diameter. This is a critical advantage over existing methods, as it allows the use of adequately refined CFD mesh to fully resolve the flow features in the boundary layers, which are critical for determining the bed shear stresses and thus the sediment motions. A number of sediment transport simulations are performed by using an in-house code lammpsFoam, a general-purpose, three-dimensional CFD—DEM solver. The number of particles used in the simulations ranges from a few hundred to a few million. Characteristics of the flow and the sediment transport, specifically including the flow velocities, Reynolds stresses, sediment transport rate, and the particle distributions in the flow, are compared with previous results in the literature [3]. Favorable agreements with the benchmark results are obtained, showing the capabilities and potentials of CFD-DEM solvers in the simulation of sediment transport.

[1] R. Sun and H. Xiao. Diffusion-Based Coarse Graining in Hybrid Continuum—Discrete Solvers: Applications in CFD—DEM. *International Journal of Multiphase Flow*, 2015. Accepted. Also available at arxiv:1409.0022. [2] R. Sun and H. Xiao. Diffusion-Based Coarse Graining in Hybrid Continuum—Discrete Solvers: Theoretical Formulation and A Priori Tests. Submitted. Also available at arxiv:1409.0001. [3] A.G. Kidanemariam and M. Uhlmann. Direct numerical simulation of pattern formation in subaqueous sediment. *Journal of Fluid Mechanics*, 750, 1-13, 2014.

Title: Modeling of Free-Surface Flow and Slamming Using Smoothed Reproducing Kernel Particle Method

Author(s): Chien-Ting Sun, Pai-Chen Guan, *Nat'l. Taiwan Ocean U.*

In the area of ocean engineering and naval architecture, the effect of slamming load is an important issue of naval structure and coastal design, because it creates large impact loading on naval structures repeatedly. The slamming can be the result of regular ship operation such as surface wave hitting ship hull, heave and pitching motion of ship, or extreme condition including underwater explosion, etc. By analyzing the loading history of vessel and offshore structure, we can observe the response of the structure and improve the survivability of naval structures. Generally, the modeling of hydrodynamics and solid mechanics are under the Eulerian and Lagrangian frameworks, respectively. The difference between frameworks increases the difficulties of coupling each other. Also, the general mesh-based methods are incapable of defining the evolvement of free surface under large deformation and suffer the mesh distortion problem. On the other hand, the meshfree methods are easier when dealing with the free-surface evolution of fluid and separation of solid body. Therefore, in this research, we develop a coupled fluid-solid program by using the Reproducing Kernel Particle method (RKPM). The RKPM can change the order of approximation and introduce enrichment for the shape function. And it also improves the drawback of boundary deficiency. Under the proposed framework, the weak-form RK formulation is used for both solid and fluid problems. The weak form of hydrodynamics formulation introduces the control volume to avoid calculating the direct derivative of shape function at the nodal position, which removes the rank deficiency and improve the stability of the numerical scheme. A surface particle identification method based on ghost layer RK gradient approach is proposed. Therefore, the free surface condition can be imposed on the surface particles to satisfy atmosphere pressure. The fluid-solid interface force is decomposed into tangent and normal direction. We applied the boundary layer theorem to calculation the average forces in the tangent direction on the boundary particles. The solid part follows the semi-Lagrangian RK formulation [1] and is developed for fragment/impact problems. Several benchmark problems are used to demonstrate the reliable and robust of coupled program. 1.Guan, P. C., Chi, S. W., Chen, J. S., Slawson, T. R., Roth, M. J., "Semi-Lagrangian reproducing kernel particle method for fragment-impact problems", INTERNATIONAL JOURNAL OF IMPACT ENGINEERING, Volume 38 Issue 12 P1033-1047, 2011,12. Keywords: reproducing kernel particle method, free surface flow, Hydrodynamic, water tank, meshfree method, Fluid-Structure-Interaction

Title: A Systematic Framework for the Prediction of Twinning in Magnesium Validated Through Large-Scale Ab-Initio Simulations

Author(s): Dingyi Sun, Mauricio Ponga, *Caltech*.

Magnesium, a hexagonal close-packed material, offers tremendous opportunities as a lightweight alternative to aluminum and steel in many engineering applications. Before such a replacement can be realized, however, one must understand its mechanisms of deformation in order to be able to design materials with greater formability than the traditionally poorly-formable magnesium. Crucial to the understanding of these deformation mechanisms is twinning - a planar defect in which the lattice on one side can be regarded as a rotation or reflection of the lattice on the other. Traditionally, twinning has been studied through a primarily experimental framework, with high-resolution TEM imaging being used as the main observational tool. These lattices are then described mathematically through a combination of non-unique lattice vectors and shuffles. Many of these mathematical descriptions, however, have been limited to pursuing only twin modes which have been experimentally confirmed. Few works have attempted to use mathematics as a means of predicting twin modes in a material. In our work, we propose a generalized framework for predicting twinning deformation modes in materials. We extend on previous works - in particular, the framework introduced by Ericksen and Pitteri - and use computations to systematically predict all possible twin modes in a given material (in our case, magnesium). We then make use of large scale ab-initio simulations with the density functional theory code developed within our group, MacroDFT, in order to form an understanding of the energetics behind these twins, identifying which ones are the likeliest to form. We then describe how we hope to use these computational findings to supplement experimental validation and possibly predict novel twin modes which have not yet been visualized in the experimental setting.

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Title: A Discrete Continuum-Coupling Approach for Predicting Anisotropic Damages in Water-Saturated Brittle Rocks

Author(s): WaiChing Sun, Kun Wang, *Columbia U.*

We develop a dual-scale model to predict the brittle behavior of water-saturated rocks under various drainage condition across length scale. In this formulation, we exploit the effect stress principle to partition stress stemming from grain contact and grain-to-grain bonding and those from fluid-solid interfaces at grain-scale. While the evolution of microstructures of solid skeleton is simulated explicitly at grain scale via discrete mechanics approach, the interaction of pore fluid and solid grain is captured at continuum scale via a mixed finite element u-p formulation. As a result, there is no need to incorporate phenomenological law to govern damage or phase field evolutions at the macroscopic continuum level. Various strategies to overcome mesh bias will be compared. Numerical examples will be used to demonstrate the accuracy and robustness of the multiscale multiphysics model.

Title: A Sweeping Window Method for Flaw Detection Using an Explicit Dynamic XFEM with Absorbing Boundary Layers

Author(s): Hao Sun, *MIT*; Haim Waisman, Raimondo Betti, *Columbia U.*

We present a sweeping window method in elastodynamics for detection of multiple flaws embedded in a large structure. The key idea is to measure the elastic wave propagation generated by a dynamic load within a smaller detecting window domain, given a sufficient number of sensors. Hence rather than solving the full structure, one solves a set of smaller dynamic problems quickly and efficiently. To this end, an explicit dynamic eXtended Finite Element Method (XFEM) with circular/elliptical void enrichments is implemented to model the propagation of elastic waves in the detecting window domain. To avoid wave reflections, we consider the window as an unbounded domain with the option of full-/semi-/quarter-infinite domains and employ a simple multi-dimensional absorbing boundary layer technique. A spatially varying Rayleigh damping is proposed to eliminate spurious wave reflections at the artificial model boundaries. In the process of flaw detection, two phases are proposed: (i) pre-analysis -- identification of rough damage regions through a data-driven approach and (ii) post-analysis -- identification of the true flaw parameters by a two-stage optimization technique. The "pre-analysis" phase considers the information contained in the "pseudo" healthy structure and the scattered wave signals providing an admissible initial guess for the optimization process. Then a two-stage optimization approach (the simplex method and a damped Gauss-Newton algorithm) is carried out in the "post-analysis" phase for convergence to the true flaw parameters. A weighted sum of the least squares, of the residuals between the measured and simulated waves, is used to construct the objective function for optimization. Several benchmark examples are numerically illustrated to test the performance of the proposed sweeping methodology for detection of multiple flaws in an unbounded elastic domain.

Title: Issues in Parallel CFD Execution on Clouds, Grids and Clusters

Author(s): Vaidy Sunderam, *Emory U.*

Parallel numerical solutions to CFD problems can be executed on different platforms, including local clusters, grids, and clouds. All platforms are now mainstream technologies in many application domains and user constituencies. However, for scientific high-performance applications in general and CFD in particular in academic and research settings, the trade-offs between cost and elasticity on the one hand, and performance and access on the other, is not always clear across these three types of platforms. We discuss our experiences with comparing cost and utility for a hemodynamics computational fluid dynamics code on these three typical platform-types available to researchers, namely IaaS clouds, grids, and on-premise local resources. To rank the tested platforms, we introduce a simple utility function describing the value of a completed computational task to the user as a function of the wait time and the cost of the computation. Our results suggest that IaaS clouds can be a convenient choice for the considered class of CFD simulations, providing a valuable tradeoff between cost and task completion time.

Title: High-Resolution Microstructural Design for Additive Manufacturing

Author(s): Krishnan Suresh, *U. Wisconsin.*

A salient feature of additive manufacturing (AM) is that the cost of fabrication, to a large extent, is independent of geometric complexity. This opens new opportunities for custom-designing parts, both at a macro and micro-level. Specifically, current AM processes can easily achieve a 100 micron resolution (or less), and thus complex multi-scale structures can be easily fabricated today. One of the challenges however is in the optimal design of such parts. An elegant and powerful design method for AM is topology optimization. The focus of this presentation is on microstructural topology optimization for additive manufacturing. The objective in microstructural topology optimization is to find locally periodic structures with desired (homogenized) macroscopic elastic or thermal behavior. The modern approach towards microstructural design is to combine continuum finite element analysis with optimization. While the theory of microstructural topology optimization is well understood, current methods can be extraordinarily expensive, taking several hours on CPU clusters. This can be detrimental to the integration of microstructural design into mainstream engineering and AM driven applications. In our research group (www.ersl.wisc.edu), we have developed highly efficient microstructural design methods [1] that can trace the theoretically optimal Hashin-Shtrikman curves for such structures. In this presentation, the computational bottle-necks in microstructural topology optimization will be identified. Then, a framework that not only eliminates these bottle-necks, but incorporates other significant improvements, will be presented. The framework is demonstrated through numerical experiments involving microstructures with millions of degrees of freedom, using multi-core CPUs and NVidia GPU. Other salient features of the proposed framework is that the underlying stiffness matrices are always well-conditioned, and multi-fold symmetry can be imposed and exploited during the optimization process. [1] K. Suresh, "Efficient Microstructural Design for Additive Manufacturing," in Proceedings of the ASME 2014 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference, Buffalo, NY, USA, 2014.

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Title: Towards Mechanics Using Quantum-Mechanics

Author(s): Phanish Suryanarayana, *Georgia Inst. Tech.*.

Ab-initio theories like Density Functional Theory (DFT) have been remarkably successful in predicting a wide range of material properties. However, the tremendous computational expense associated with these first-principles calculations severely restricts the size of systems that can be studied. In fact, routine simulations using DFT are typically limited to hundreds of atoms. As a result, most mechanics-related problems of interest are currently intractable. Indeed, even the relatively 'simple' problem of accurately determining the nature of a dislocation's core is a challenging one. In this talk, previous and current efforts of the speaker to overcome the aforementioned limitations will be presented.

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Title: An Improved Compressible, Multi-Phase, Semi-Implicit Method with Moment of Fluid Interface Representation

Author(s): Mark Sussman, Matthew Jemison, M. Yousuff Hussaini, *Florida State U.*; Marco Arienti, *Sandia Nat'l. Lab.; Livermore.*

We present improvements made to our algorithm, "Compressible, Multiphase Semi-Implicit Method with Moment of Fluid Interface Representation" first reported in *Journal of Computational Physics* (2014). The improvements enable more accurate simulation of compressible multiphase flows, but with the same cost. Examples are presented for high pressure atomization of liquid in gas and for multiphase problems consisting of materials with large viscosity. As with our 2014 method, our improved method is asymptotically preserving, conservative, simulates materials with disparate material properties, and does not require Riemann solvers.

Title: Biomechanical Modeling of Breast Shape and Deformation After Mastectomy Reconstruction Surgery

Author(s): Alok Sutradhar, *Ohio State U.*

An effective treatment for invasive cases of breast cancer is to remove the entire breast, commonly known as mastectomy. After mastectomy surgery, women often feel anxious, depressed, and even “being disabled” due to the loss of the breasts. Reconstructing the breasts for women help them recover their body forms, confidence, femininity, and functionality. Currently, there is no tool for surgeons to preplan the breast reconstruction which results in poor outcome and, typically it takes 3 to 4 iterations to get acceptable results adding more trauma and anxiety for the patient. In this work, a biomechanical model is developed to predict the breast deformation and shape after the reconstruction. Patient-specific finite element models are generated using 3D surface scanners and other imaging modalities. The skin plays a critical role in the breast shape and deformation. Special considerations are given to the modeling of the breast skin. The mechanical properties of the skin are obtained experimentally. The biomechanical model is assessed for breast shape changes in several states of breast deformation due to change in patient positions and by simulating simple surgical procedures. The initial results show good promise towards developing a breast surgery simulation framework.

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Title: Multi-Scale Seamless Domain Method for Linear and Nonlinear Analyses of Heterogeneous Materials

Author(s): Yoshiro Suzuki, *Tokyo Inst. Tech.*

A new meshfree numerical analysis, termed the seamless domain method (SDM) [1], is applied in a multiscale technology. The SDM requires only coarse-grained points and does not need a stiffness equation, mesh, grid, cell, or element. The SDM is composed of two analyses. The first is a microscopic analysis of local simulation domain to obtain shape functions for interpolation of dependent-variable distributions and influence coefficients for calculation of interaction between the points. These allow an SDM solution to represent a heterogeneous material without homogenization. The second step is a macroscopic analysis of a seamless global domain without mesh or grid. The special functions obtained in the first step are used in interpolating the continuous dependent-variable distribution in the seamless global domain whose gradient is also continuous everywhere. The SDM would give a quite accurate solution for domains with strong boundary effects, anisotropic and heterogeneous materials, and isotropic homogeneous fields. In this study, we applied the SDM to analyses of fiber composite materials. Various kinds of numerical examples illustrated that the method worked out linear elastic fields and nonlinear steady-state temperature fields. Every SDM solution using only a few hundreds of points was as accurate as that from conventional finite element analysis using more than hundreds of thousands of node points.

Title: Effect of Elevated Intracranial Pressures on Cerebral Aneurysm: A Fluid-Structure Interaction Study

Author(s): Hasson Syed, Vinu Unnikrishnan, Semih Olcmen, *U. Alabama.*

Raised intracranial pressures (ICP) are one of the major consequences in majority of neurosurgical and neurological patients. The changes in pressure inside the skull (ICP) is commonly attributed to the volume changes in one or more of the constituents contained in brain mainly cerebrospinal fluid, blood in the cerebral vasculature and the brain. The compensatory mechanisms of the brain such as the reduction of volume of cerebrospinal fluid or intracranial blood keeps the ICP stable in a healthy adult. The normal ICP in a supine healthy adult ranges between 7.0 and 15.0 mmHg (0.09Kpa-1.9Kpa). Often increase in ICP is attributed to many causes such as the excessive accumulation of cerebrospinal fluid due to cerebral edema (swelling of brain), as a result of traumatic brain injuries (TBI) or mass effect from a lesion (tumor) etc. High ICPs can lead to severe brain disabilities resulting from brain stem compression and impaired blood circulation within the brain. Intracranial bleeding (hemorrhage) can also take place when the blood vessel within the skull leaks because of TBI or rupture of cerebral aneurysms (dilatation or ballooning of the arterial wall) due to high ICP. Hence, understanding the mechanics of the arterial wall plays a significant role in the rupture or enhancement of the aneurysm. Understanding the flow behavior through cerebral arteries and aneurysms helps in understanding the factors that can lead to onset of rupture of the aneurysm and ways to mitigate these effects. Wall Shear Stress (WSS), is an important parameter for the estimation of progression of cerebral arterial damages, and typically varies with the pulsatile nature of blood flow. The variation of WSS with changes in the ICPs can be a good indicator of stress experienced by the arterial wall with and without aneurysm. In this work, fully coupled fluid structural interaction simulations on the cerebral artery and aneurysm are carried out to investigate the effect of intracranial pressure waveforms on the wall shear stress distribution and displacement of the cerebral artery or aneurysm. Three different varying ICP waveforms and three constant ICP profiles acting on the cerebral arterial wall and on cerebral aneurysm are analyzed in this study. The changes in the WSS with flow rate coupled with changes in ICP will be presented, together with the effect of varying properties of the arterial wall.

Title: Computational Modeling of Cardiac Looping

Author(s): Yunfei Shi, *Washington U.* ; Larry Taber, *Washington U.*.

In the early embryo, the morphogenetic process of cardiac looping transforms the straight heart tube (HT) into a curved tube that resembles the shape of the future four-chambered heart. Despite intensive study for nearly a century, the physical forces that drive looping have remained poorly understood. Recent work, however, has shed new light on this complicated problem. For example, recently published data suggests that differential hypertrophic growth may play a role in looping (Soufan et al., 2006). Prior to this study, experimental measurements of mitotic rates had seemingly eliminated differential growth as a major factor in looping, as it has commonly been thought that the heart grows almost exclusively via hyperplasia before birth and hypertrophy after birth. Considering these new findings, we propose a relatively comprehensive hypothesis for the mechanics of the first phase of looping, termed c-looping, as the HT bends and twists into a c-shaped tube (Shi et al., 2014a; 2014b). According to this hypothesis, differential hypertrophic growth in the myocardium supplies the main forces that cause the heart tube to bend, while regional growth and contraction in the omphalomesenteric veins (primitive atria) and compressive loads exerted by the splanchnopleuric membrane drive rightward torsion. A computational model based on realistic embryonic heart geometry is used to test this hypothesis. The behavior of the model is in reasonable agreement with available experimental data from control and perturbed chick embryos. The results also suggest, however, that several other mechanisms contribute secondarily to normal looping, and we speculate that these mechanisms play backup roles when looping is perturbed. These results should shed new light on the mechanisms that drive this crucial morphogenetic process. References Shi, Y., Yao, J., Xu, G., Taber, L.A., 2014a. Bending of the looping heart: differential growth revisited. *J Biomech Eng* 136, 081002. Shi, Y., Yao, J., Young, J.M., Fee, J.A., Perucchio, R., Taber, L.A., 2014b. Bending and twisting the embryonic heart: a computational model for c-looping based on realistic geometry. *Front Physiol* 5, 00297. Soufan, A.T., van den Berg, G., Ruijter, J.M., de Boer, P.A., van den Hoff, M.J., Moorman, A.F., 2006. Regionalized sequence of myocardial cell growth and proliferation characterizes early chamber formation. *Circ Res* 99, 545-552.

Title: An Adaptive Parametrized-Background Data-Weak Approach to State Estimation

Author(s): Tommaso Taddei, James Penn, Masayuki Yano, Anthony Patera, *MIT*.

We present an adaptive Parametrized-Background Data-Weak (PBDW) formulation for state estimation data assimilation problems modelled by parametric PDEs. PBDW combines in a variational fashion a background (prior) space, which approximates the solution manifold associated with the parametric PDE, and M experimental observations. The adaptive procedure exploits a novel a posteriori observation-based error estimator to refine the prior space using historical data-assimilation solutions. Special attention is given to the choice of the inner product used in the variational formulation, and to the connection of the PBDW approach with Radial Basis Function (RBF) interpolation. We present a priori and a posteriori theory for the state estimation error, and we numerically evaluate our method through a frequency domain resonator problem and a transient thermal patch problem.

Title: Cauchy-Born ANSYS

Author(s): Ellad Tadmor, Jiadi Fan, Ryan Elliott, *U. Minnesota.*

The Cauchy-Born (CB) rule relates a continuum deformation gradient to the motion of atoms in an underlying crystal structure. This kinematics is used to define the constitutive response in the continuum region of the quasicontinuum method. Here we develop a CB-based constitutive model as an external user material subroutine (USERMAT) to the commercial finite element code ANSYS. This enables users to perform 3D finite deformation ANSYS simulations using an atomistically-based single-crystal constitutive model that correctly describes material nonlinearity and phenomena such as phase transformations and lattice invariant deformations. The CB USERMAT is compliant with the Knowledgebase of Interatomic Models (KIM) application programming interface (API), which means that it can work with any interatomic potential in the KIM repository at <https://openkim.org>. Some sample ANSYS applications using the CB model will be shown.

Title: Regularity and Connectivity Conditions of a Generalized Particle-Based Method for Partial Differential Equations

Author(s): Daisuke Tagami, Yusuke Imoto, *Kyushu U.*

To obtain error estimates of particle-based methods for partial differential equations, we present regularity and connectivity conditions of a generalized particle-based method for partial differential equations, which is one of alternative formulations of particle-based methods and which includes not only SPH (Smoothed Particle Hydrodynamics) but also MPS (Moving Particle Semi-implicit) by taking appropriate particle volumes and reference functions. There are few studies for error estimates of particle-based methods (SPH, MPS, and others); we can find error estimates of SPH for conservation laws in Mas-Gallic--Raviart [2] and Moussa--Via [3]. However, there are some differences between SPH in [3] and conventional ones; for example, particle volumes are defined by the Jacobian based on the flow field, and it is difficult to extend to practical numerical computations. We can also find truncation error analysis in Ishijima--Kimura [1]. They introduce some indicators to define the properties of particle distributions. However, we can not compute actually the values of indicators, and it is also difficult to extend to practical numerical computations. In this paper, at first, we consider numerical analysis of the generalized particle-based method for Poisson equations. By introducing regularity and connectivity conditions on particle distributions and influence radius used in the interpolants and the approximate operators, we obtain the unique solvability and the discrete maximum principle of approximate Poisson equations. These facts lead the error estimates of the generalized particle-based method for Poisson equations, which are optimal in the sense that its have the same orders as the convergence orders of interpolants with respect to the influence radius. Next, we analyze heat equations approximated by the generalized particle-based methods in space and the backward Euler method in time. Under the regularity condition and the restrictions on the influence radius and time increments, we also establish optimal error estimates. Moreover, some numerical results are shown. The numerical convergence rates of errors coincide well with the theoretical ones. [1] Ishijima, K and Kimura, M. (2010): Truncation error analysis of finite difference formulae in meshfree particle methods, *Trans. Japan Soc. Indust. Appl. Math.*, 20, pp.165--182. [2] Mas-Gallic, S. and Raviart, P.-A. (1987): A Particle Method for First-order Symmetric Systems, *Numer. Math.*, 51, pp.323--352. [3] Moussa, B.B. and Vila, J.P. (2000): Convergence of SPH Method for Scalar Nonlinear Conservation Laws, *SIAM J Numer. Anal.*, 37, pp.863--887.

Title: A Thermal Noise Reduction Technique for Atomic Structure Analysis

Author(s): Akiyuki Takahashi, Koya Nakamura, Kazuki Takahashi, *Tokyo U. Science*; Akiyoshi Nomoto, *Central Rsch. Inst. Electric Power Ind.*.

Thermally activated process of defects generally controls the material deformation behavior under finite temperature conditions. The atomistic mechanism can be investigated using the molecular dynamics simulation with an appropriate interatomic potential. From the results of molecular dynamics simulations, say atomic positions, the underlying lattice structure must be extracted for clarifying the atomistic structure and behavior of defects. However, in the results, the position of atoms is displaced from the underlying lattice point due to a strong influence of thermal vibration. Therefore, in order to investigate the atomic mechanism of defect behavior using molecular dynamics simulations, it is very important to develop a numerical technique for analyzing the lattice structure from thermally vibrated atomic positions. This paper presents a new numerical technique for reducing thermal noise in molecular dynamics simulation results of atomic structure under finite temperature conditions. In the technique, a marker mass is added as a new degrees of freedom in the molecular dynamics simulation, which is connected to an atom with a spring, and can move only in the immediate vicinity of the underlying lattice point. Using the position of marker mass, the accuracy of the atomic structure analysis using either common neighbor analysis (CNA) or central symmetry parameter (CSP) can be drastically improved even under very high temperature condition. As a benchmark test of the technique, we simulated atomic behavior in a perfect bcc crystal lattice under various temperature conditions. Then, we monitored the distance between each marker mass and each corresponding lattice point. The results clearly show that the marker mass position is relatively close to the lattice point rather than atomic position even under very high temperature condition. Then, we simulated the edge dislocation behavior under a temperature condition, and analyzed the lattice structure using both CNA and CSP. The results show that, if we analyze the lattice structure using atomic positions, the CNA and SCP provide a lot of misunderstanding of lattice structure due to the influence of thermal vibration. However, if we use the position of marker mass, the edge dislocation core structure can be extracted from the molecular dynamics simulation results without any misunderstanding. Therefore, the use of marker mass enables us to accurately analyze the defect structure in the molecular dynamics simulation results under finite temperature conditions.

Title: Finite-Cover-Based FSI Analysis with Tsunami Impact Loading

Author(s): Shinsuke Takase, Shuji Moriguchi, Kenjiro Terada, Mayu Muramatsu, *Tohoku U.*

We propose a new fluid-structure interaction (FSI) analysis method, in which the finite cover method (FCM) is employed for interface capturing to properly evaluate the impact loading caused by tsunami. The stabilized finite element method is applied to solve the Navier-Stokes equations with a spatially fixed FE mesh, over which the Lagrangian meshes of structures are placed independently. In this study, the structures are assumed to be rigid bodies, and their motions and mutual contact are simulated with the discrete element method (DEM). Then, the key ingredient of the proposed method to accurately evaluate the impact loading caused by tsunami is the FCM, which enables us to realize appropriate discretization around the interfaces defined as intersections of the Eulerian mesh for fluids and the Lagrangian meshes for the rigid bodies. The continuity conditions of velocity and stress vectors at each interface are imposed with the penalty method. Also, we carry out the free surface flow simulations, for which the SUPG method is employed to discretize the Navier-Stokes equation. To capture the complex free surface motion such as breaking waves in case of tsunami impact, we apply the phase-field modeling with the conservation-modified Allen-Cahn equation. The concrete modeling procedure of the proposed method is given as follows: First, the domains of rigid bodies, which can be of arbitrary shapes, are discretized with FE meshes as if they were deformable solids. Then, rigid particles for the DEM are placed for contact decision on the surface of the generated meshes. Second, the generated meshes for the structures are superimposed onto a spatially fixed mathematical mesh, which is set up independently of the domains of structures. Third, the level-set functions are introduced to determine the outer and inner sides of the domains of structures. Fourth, after extracting the finite elements in the Eulerian mesh for fluids that intersect with the boundaries of the structures, we determine the location of the interface inside each of the extracted elements with the help of the pre-defined level-set functions. Finally, the meshes for the extracted fluid domain facing the structures are re-generated. After verification analyses are carried out in comparison with experimental data, several representative numerical examples are presented to demonstrate the promise and performance of the proposed FSI analysis method. In particular, a simple FSI problem is solved to simulate the collapse process of structures by the tsunami impact loading and the subsequent flow involving broken members.

Title: Space-Time Interface Tracking in Fluid Mechanics Computations with Contact Between Moving Solid Surfaces

Author(s): Kenji Takizawa, Shohei Asada, *Waseda U.*; Tayfun Tezduyar, Austin Buscher, *Rice U.*

We present a space–time (ST) interface-tracking (moving-mesh) method [1] that gives us interface-tracking accuracy in fluid mechanics computations with contact between moving solid surfaces or other topology change (TC). The method is a new version of the Deforming-Spatial-Domain/Stabilized ST (DSD/SST) method [2-6], and we call it ST-TC. With this method, fluid mechanics computations, even in the presence of contact between the moving solid surfaces, can be done without compromising accurate representation of the flow patterns near the fluid–solid interfaces. This enables us to accurately model challenging problems such as heart valves with contact when the valve leaflets close. The method includes a master–slave system that maintains the connectivity of the "parent" mesh when there is contact between the moving interfaces. It is an efficient, practical alternative to using unstructured ST meshes. We explain the method with conceptual examples [1], present 2D test computations [1] with models representative of the classes of problems we are targeting, and 3D computations with heart valve models [7]. We present computations for two models: an aortic valve with coronary arteries and a mechanical aortic valve. These computations demonstrate that the ST-TC method can bring interface-tracking accuracy to fluid mechanics problems with TC, and can do that with computational practicality. REFERENCES [1] K. Takizawa, T.E. Tezduyar, A. Buscher and S. Asada, "Space-Time Interface-Tracking with Topology Change (ST-TC)", *Computational Mechanics*, 54 (2014) 955-971. [2] T.E. Tezduyar, "Stabilized Finite Element Formulations for Incompressible Flow Computations", *Advances in Applied Mechanics*, 28 (1992) 1-44. [3] T.E. Tezduyar, "Computation of Moving Boundaries and Interfaces and Stabilization Parameters", *International Journal for Numerical Methods in Fluids*, 43 (2003) 555-575. [4] T.E. Tezduyar and S. Sathe, "Modeling of Fluid-Structure Interactions with the Space-Time Finite Elements: Solution Techniques", *International Journal for Numerical Methods in Fluids*, 54 (2007) 855-900. [5] K. Takizawa and T.E. Tezduyar, "Multiscale Space-Time Fluid-Structure Interaction Techniques", *Computational Mechanics*, 48 (2011) 247-267. [6] K. Takizawa and T.E. Tezduyar, "Space-Time Fluid-Structure Interaction Methods", *Mathematical Models and Methods in Applied Sciences*, 22, 1230001 (2012). [7] K. Takizawa, T.E. Tezduyar, A. Buscher and S. Asada, "Space-Time Fluid Mechanics Computation of Heart Valve Models", *Computational Mechanics*, 54 (2014) 973-986.

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Title: State-of-the-Art and Overview of Advances in "Integrators" and Framework of Implicit/Explicit Algorithms/Designs for Multiphysics Applications

Author(s): Kumar Tamma, Masao Shimada, *U. Minnesota.*

Recently, we have developed under the umbrella of "isochronous time integrators [Integrators]" representing the use of the "same time integration framework/architecture" novel designs for first/second order ODE transient/dynamic systems for the general class of LMS methods that not only encompass most of the research to-date developed over the past 50 years or so, but additionally encompasses more new and novel schemes with improved physics such as energy-momentum or symplectic-momentum conservation and other optimal attributes with/without controllable numerical dissipation [1-2]. Each engineering multi-physics application has its own emphasis and analysis requirements; wishful thinking is that a wish list of desired attributes by the analyst to meet certain required analysis needs is desirable. Optimal design developments of algorithms are not trivial; and alternately, how to foster, select, and determine such optimal designs for a targeted application if such an optimal algorithm does not readily exist, is a desirable goal and challenging task. Under the notion of Algorithms by Design and the theoretical basis emanating from a generalized time weighted residual philosophy, we provide recent advances in utilizing the same unified Integrator framework and wide variety of embedded implicit/explicit architecture of algorithms and designs for general coupled multi-physics/multi-disciplinary applications. Such analysis can simultaneously involve algorithms for first-order systems (sub-cases, Crank-Nicholson, Gear, MacCormack's method and so on including more new and optimal designs encompassing both implicit and explicit schemes) or second-order systems (sub-cases, Newmark, HHT, WBZ and many others, and more new and optimal algorithms such as optimal U0-V0 with controllable numerical dissipation) for applicability to thermal-structural, fluid-structure, type interactions and the like. Individual disciplines or multi-physics applications may entail mixed implicit/explicit, implicit-implicit, or explicit-explicit formulations within the same physical mesh; here we explore two schools of thought, namely, the sense of subcycling as an ODE approach, or alternately as subdomain integrators that are instead treated as a DAE approach. All formulations within the "Integrator framework of mixed implicit/explicit designs" yield second-order time accuracy in all kinematic and algebraic variables. Under the umbrella of a single unified architecture, the Integrator framework is envisioned as the next generation toolkit; and illustrative examples are highlighted as well. References: J. Har and K. K. Tamma; "Advances in Computational Dynamics for Particles, Materials, and Structures", John Wiley and Sons, Inc., July 2012. K. K. Tamma; "The Time Dimension: Integrators and Implicit/Explicit Framework for Computational Dynamics," COMPDYN 2013, Kos Island, Greece, June 2013 (Plenary Lecture).

Title: Concurrent Multi-Scale Modelling of Amorphous Materials

Author(s): Vincent Tan, *Nat'l. U. Singapore.*

We present a multiscale approach to modelling amorphous materials whereby atomistic scale domains coexist with material continuum domains. The atomistic scale domains faithfully predict severe deformation while the continuum domains allow the computation to scale up the model without incurring excessive computational costs associated with fully atomistic models. While various multiscale approaches methods have been formulated, few have been applied to model amorphous materials. The method presented here uses an amorphous cell as building blocks for amorphous materials. Rather than solving for the position of all the molecules of the constituent amorphous cells, displacements of the vertices of the cells (a.k.a. nodes) are the unknowns. The molecular displacements are then recovered from the nodal displacement through a mapping function, T . The proposed method allows regions where atomistic details are important to be modelled by classical atomistics simulation. The connection between the amorphous cell region and the atomistics region is seamlessly effected by augmenting the T transformation matrix. The distinction of the proposed method from other multiscale method lies in the T transformation matrix. With many other methods, an arbitrary function to extract the displacements of molecules from the displacements of a reduced number of representative atoms is required. Currently, the most common extraction functions are interpolation functions. However, for an amorphous material, molecular displacements cannot be expected to follow or even approximate interpolated values of selected nodes or atoms. The T matrix is derived in recognition of this shortcoming to extract the molecular displacements according to the modes of deformation of the cells which turn out to be very different from simple linear interpolation. We have shown that the proposed method gives molecular displacements that are indistinguishable from MD simulations for up to 5% strain whereas interpolation functions give rise to considerable errors at even 0.2% strain for amorphous materials.

Title: Large-Scale Earthquake Response Analysis of Soil and Structure Based on Solid Finite-Element Method

Author(s): Seizo Tanaka, Tsuyoshi Ichimura, Muneo Hori, Maddeggedara Wijerathne, *U. Tokyo.*

The structures must have an enough performance against the external forces caused by natural disaster such as earthquakes. The infrastructures and important structures such as the bridges, highways, tunnels, high-rise buildings, and power plant buildings must be designed prudently and requires accurate assessment. To estimate a behavior of structures during earthquakes, the dynamic soil-structure interaction should be considered. The accurate evaluation of seismic response of soil-structure by numerical simulation with high-fidelity model requires high resolution to both spatial and temporal domain. The size of domain for soil should be huge; on the other hand, the resolution of structure model should be high. Numerical simulation with high resolution needs significant amount of computational time and memory usage. The development of parallel computer architecture and fast network system in recent years has dramatically been realizing the large-scale simulations. Numerical analysis will be a substitute, if it able to estimate the damage of structure. For requires as mentioned above, we have to compute the large-scale problems on the large computer system. In this presentation, we report large-scale seismic response analysis to estimate the structural damage. For the problem of the seismic soil-structure interaction analysis based on time-dependent linear elastic body finite element method, we implemented high performance computing techniques such as MPI/OpenMP hybrid parallelization, multi-grid/multiple-precision preconditioned CG method, to reduce the computational cost which is able to solve high fidelity model of a structure subjected to the ground motion. Also, we have implemented the developed code onto K supercomputer, and carried out it.

Title: Multi-Scale Segmentation of a Unified Creep-Fatigue Crack Growth Model

Author(s): K. K. Tang, *Tongji U.*

A unified multiscale creep-fatigue crack growth model $da/dN-\Delta S$ is proposed based on the volume energy density. Creep effects are included by incorporating mean stress in the ΔS model. Change of R ratios lead to the selective transitional functions and mutual interacting of creep and fatigue. Effects of creep and fatigue are thus unified in one crack growth model. The behaviors of non-equilibrium and non-homogeneity (NENH) are reflected through the three transitional functions. Multiscaling has outgrown the applicability of stress intensity factor K or the energy release rate G. They were thought to be the crack driving force for characterizing the monoscale fracture property whereby microscopic effects are excluded. The energy-based ΔS model overcomes the monoscale limitation. The NENH behavior of FCG can be segmented into three stages including pico-nano, nano-micro and micro-macro, each characterized by their unique crack tip singularities that are determined by the Fadde eigenfunction method as 1 for the nanocrack, 0.75 for the microcrack and 0.5 for the macrocrack. The different singularities allude to the energy dissipation characteristics at the different scales. Transitionalized crack length (TCL) is derived from the ΔS model while fictitious crack length (FCL) is generated from the ΔK model. The two models provide different physical interpretations of already measured test data of 2024-T3 Al sheets. The micro-macro test data for crack lengths 3-55mm can be used to derive crack data in the nano-micro range or the range of macro-large. TCLs from the proposed multiscale model not only have a better agreement with the test data, but also offer an explanation for the crack growth in fatigue test specimen with edge restriction. Key words: NENH; TCL; FCL; Volume energy density; transitional functions

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Title: Isogeometric Boundary Element Methods

Author(s): Matthias Taus, Gregory Rodin, Thomas Hughes, *UT Austin*.

Isogeometric Boundary Element Methods have numerous advantage over conventional ones because the underlying approximations exhibit additional smoothness. As a result, one can develop methods featuring (i) higher-order collocation schemes, (ii) systems of linear algebraic equations with problem-size independent conditioning, and (iii) very accurate numerical integration schemes. In addition, unlike conventional methods, Isogeometric Boundary Element Methods can be subjected to patch testing. We will present several numerical examples which feature essentially machine precision computations

Title: Novel Image Processing Pipeline for Dermoscopic Images

Author(s): Zhen Ma, Joao Tavares, *U. Porto*.

Dermoscopy is widely used to diagnose skin lesions, but the accuracy of this technique largely depends on the dermatologist's experience. Hence, image processing techniques are demanded in order to make less subjective and time consuming. The ABCD rule, which is based on the asymmetry, border, color and diameter of the lesion, is commonly accepted to classify the lesion as a melanoma or not. The application of this rule is usually divided into three main steps: identification of the lesion in the input image, i.e. lesion segmentation, feature extraction and classification. Here, we propose a new image processing pipeline developed to assist this procedure. In the pipeline developed, an approach based on a deformable model [1] and on fusion of the information attained from different color channels is used to segment the lesion under analysis. Then, with the boundary of the lesion detected, the shape and color of the lesion is analyzed and quantitative measures based on the ABCD rule are computed. The classification step is carried out using computational classifiers; in particular, support vector machine and neural network based classifiers. Three datasets containing significant numbers of representative dermoscopic images acquired under different imaging conditions have been used to validate the pipeline proposed and compare the classifiers used. The experimental results obtained are very promising. Acknowledgements 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 post-doc grant: SFRH/BPD/97844/2013. References [1] Ma, Z., Tavares, J.M.R.S. (in press): A novel approach to segment skin lesions in dermoscopic images based on a deformable model. IEEE Journal of Biomedical and Health Informatics. DOI: 10.1109/JBHI.2015.2390032.

Title: Adjoint-Based Posteriori Error Estimation for Complex Systems

Author(s): Simon Tavener, *Colorado State U.*

Finite element methods are well-established and popular techniques for solving systems of partial differential equations. A priori analyses of finite element methods seek to establish error bounds in appropriate norms and to determine rates of convergence with mesh refinement. Adjoint-based a posteriori analyses seek to estimate the error in a functional of the solution (a “quantity of interest”) for a given numerical calculation. Systems of interest in science and technology commonly involve multiple physical processes which evolve on distinctly different time scales, and model parameters and even computational domains which are uncertain. Further, specific numerical approaches such as finite volume methods or explicit time integration techniques may be customary within particular scientific communities. The goal of this work is to use mathematically appealing adjoint-based a posteriori ideas to develop accurate a posteriori error estimates for a range of computational problems encountered in practice, and, where possible, to separately estimate the multiple sources of error in order to construct adaptive computational strategies. Examples of different solution techniques that have been addressed include operator decomposition in space and in time, and parallel solution strategies. Examples of different discretization techniques studied include a cell-centered finite volume method, explicit time integration methods and IMEX schemes.

Title: Non-Invasive Assessment of Coronary Artery Disease Using Image-Based Computational Fluid Dynamics

Author(s): Charles Taylor, *HeartFlow, Inc.*

Currently, the gold-standard for assessing the functional significance of coronary artery disease, fractional flow reserve (FFR) involves invasive measurement of pressure in the coronary arteries at the time of diagnostic cardiac catheterization. Given the strength of evidence on the clinical benefit of measured fractional flow reserve, there is a strong motivation to attempt to obtain this data noninvasively. FFRCT is a noninvasive technology whereby patient-specific models of blood flow are constructed from coronary CT angiography (cCTA) data and used to provide data to physicians related to the functional significance of coronary artery disease. FFRCT requires an accurate segmentation of the coronary artery lumen from cCTA data, but additionally, it leverages established biologic principles relating form (anatomy) to function (physiology). Finally, FFRCT exploits recent advances in computational fluid dynamics to solve the governing equations of blood flowing in the coronary arteries. FFRCT has been evaluated against measured FFR data in over 600 patients in three diagnostic accuracy trials to date. Most recently, the NXT trial has demonstrated accuracy against measured FFR data in 254 patients and 484 vessels not only significantly exceeding that of cCTA alone, but superior to that reported for any other noninvasive diagnostic test when compared to measured FFR as the reference standard. In a demonstration of the expected clinical use of the technology, FFRCT correctly reclassified 68% of coronary CTA false positive patients and 67% of coronary CTA false positive vessels as true negatives. The clinical use of this technology could substantially improve the identification of patients that would benefit from coronary stenting and hence should be referred to invasive cardiac catheterization. Clinical trials examining the impact of FFRCT on clinical outcomes and costs are underway. FFRCT is currently being used for clinical decision making in the United States, Europe and Japan.

Title: Plastic Strain Driven Stochastic Volume Elements for Polycrystalline Materials

Author(s): Kirubel Teferra, Lori Graham-Brady, *Johns Hopkins U.*

The sought-after virtual design environment to engineer materials with tailored properties requires unprecedented collaboration among experimentalists, modelers, materials scientists, and mechanicians to better understand fundamental mechanisms governing material behavior and structural performance. Research activities toward the goal of establishing the so-called process-structure-properties relationship involve experimentally characterizing and testing microscale specimens along with developing explanatory theories and associated numerical methods for simulation. An important aspect of this initiative is to develop tools to better understand the reliability of predictions due to uncertainties and errors associated with modeling, such as mechanical properties and microstructure morphology, as well as experimental characterization and testing, such as noisy and limited data. This talk aims to address one aspect toward improving the reliability of model-based predictions, namely, the variability of mechanical response due to the randomness and representation of morphology. The performances of three tessellation models representing polycrystalline microstructures are evaluated by comparing the discrepancies between feature statistics and mechanical response with respect to a 3D dataset of a reconstructed microstructure specimen obtained by EBSD-FIB serial sectioning. The comparison is done by first obtaining the best-fit sample per tessellation model to the data, which consequentially provides a quantitative measure of the extent to which a tessellation model is capable of representing a particular material's microstructure. Secondly, tessellation model parameters are represented by a marked point process random field model, for which simulation algorithms exist. Through Monte Carlo simulation, samples of statistically equivalent microstructures are generated consistent with target marginal distributions and some second-order statistics of the tessellation parameters, which have been empirically obtained from the best-fit sample. Using the computationally efficient FFT fixed-point iteration scheme in conjunction with phenomenological crystal plasticity constitutive models, the variability of mechanical response due to morphological randomness is quantified. One implication of this work is an improved understanding of the size of the representative volume element for polycrystalline microstructures from the extrapolation of simulations of stochastic volume elements.

Title: Microstructure Change and Interface Motion As Problems of Evolving Material Configurations

Author(s): Gregory Teichert, Krishna Garikipati, *U. Michigan.*

The evolution of material configurations involving an interface between different microstructures is examined in a continuum mechanical setting. We consider three material states: the initial material configuration, the current material configuration, and the current deformed state. A configurational placement field describes the current material configuration in terms of the initial material configuration. Equilibrium states can be found by considering variations on the current material configuration. The resulting conditions for equilibrium depend on the Eshelby stress tensor. This suggests that far from equilibrium, the velocity of the interface between the microstructures can be written as a function of the Eshelby stress tensor. We model the motion of the interface using the level set and finite element methods. An example computation demonstrates the evolution of the interface to a steady state and its interaction with the deformation of the body. References: Garikipati, et. al., "Biological remodelling: Stationary energy, configurational change, internal variables and dissipation". J. of the Mech. and Phys. of Solids, 2006. Gurtin, Morton E., Configurational forces as basic concepts of continuum physics. New York:Springer, c2000.

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Title: Large-Eddy Simulation with Near-Wall Modeling Based on Weakly Enforced No-Slip Boundary Conditions

Author(s): Andres Tejada-Martinez, Roozbeh Golshan, *U. South Florida*; Yuri Bazilevs, *UC San Diego*.

Weakly enforced no-slip wall boundary conditions are re-visited in the context of large-eddy simulations (LES) with near-wall modeling. A new formulation is proposed in the framework of weakly enforced no-slip conditions that is better aligned with traditional near-wall modeling approaches than its predecessors by taking into account the under-resolved viscous wall shear stress. The new formulation is tested on a turbulent open-channel flow at Reynolds number 395 based on friction velocity and channel half-height. The computations are performed using the residual-based variational multiscale (RBVMS) formulation of LES, discretized using quadratic NURBS (non-uniform rational B-splines). The new near-wall model formulation gives more accurate results for the mean flow and velocity fluctuations than its older versions, while exhibiting better numerical stability than traditional near-wall modeling techniques.

Title: Stochastic Characterization of Geometrical and Material Uncertainties in Simulation of Brain Mechanics

Author(s): Sonjoy Das, Therence Temfack, *U. Buffalo.*

Traumatic brain injury (TBI) is a leading cause of death and disability, and poses a serious health, economical, and social problem worldwide. Given the tremendous advancement of computing capability and cutting edge imaging techniques, modeling and simulation of brain mechanical response to head impact can provide insightful understanding about TBI. However, the modeling and simulation are often plagued by limited experimental information (both in terms of measurement resolution as well as limited samples/specimens) and modeling idealization. The goal of the current work is to characterize such limited information and modeling idealization within a probabilistic framework. A three-dimensional (3D) brain finite element (FE) model consists of geometrical features, anatomical features (e.g., skull, white and gray matter, blood vessels, cerebrospinal fluid, etc.), constitutive material parameters, loading, boundary condition, and interaction mechanism between different regions. The geometrical and anatomical features are typically gleaned from a database of two-dimensional (2D) images, while loading and material parameters are estimated from controlled mechanical testing. The boundary conditions and interaction mechanism, on the other hand, are often idealized. Significant variations in experimentally characterized material parameters can be found in the existing literature. The quality and credibility of a deterministic 3D FE model is evidently restricted after a certain extent by the finite measurement resolution, lack of sufficient experimental data and modeling approximations. To address this issue, a stochastic brain model accounting for the effects of variations in geometrical and anatomical features, constitutive material parameters, loading, boundary conditions, and interaction mechanism will be presented. The proposed stochastic model will be useful to cross-validate the probabilistic model predictions against experimental data (if and when available).

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Title: Calibration and Forward Uncertainty Propagation of Turbulence Models for Coarse-Grid, Large-Eddy Simulation

Author(s): Jeremy Templeton, *Sandia Nat'l. Lab.*

Large-eddy simulation (LES) holds the middle ground in computational fluid dynamics approaches between high-fidelity (direct numerical simulation) and low-fidelity (Reynolds-averaged Navier-Stokes) methods. While it has proven useful for scientific investigations of complex flows, its impact on the engineering process has been limited due to the difficulty existing LES turbulence models have producing the necessary stresses when coarse grids are used. Most existing models are derived by assuming isotropy of the fluctuations or grid spacing on the order of the inertial range, both of which are violated in many engineering applications. In order to assess the potential of using existing models in complex flows with modest grids, we present calibration strategies that can inform model parameters from data. This presentation overviews multiple strategies to calibrating turbulence model parameters. First, we show the results of an approach predicated upon low-pass filtering highly resolved turbulence data consistent with the mathematical foundations of LES. Two approaches to Bayesian calibration are considered: 1) a presumed error model (PEM) using an additive Gaussian discrepancy term, and 2) an embedded error model (EEM) which assumes the parameters can be represented by a polynomial chaos expansion. Both approaches produce parameters that are dependent on the filter width, suggesting the underlying model form is not necessarily appropriate for this application. While the EEM approach is shown to capture a greater range of uncertainty, neither approach produces uncertainty bounds such that predictions fall within the range of validation data due to the coarse grids that are used. A second calibration strategy informs the model parameters based on their ability to predict bulk engineering quantities. This approach results in optimal parameters far from their expected/literature values, demonstrating that existing models can be used to predict some quantities of interest if they are sufficiently modified. However, prediction requires an understanding of how model parameters vary with grid spacing and flow regime. We conclude with a discussion of how to incorporate this information into the calibration process. Sandia National Laboratories is a multiprogram 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. Funding for this work was provided by the Laboratory Directed Research and Development (LDRD) at Sandia National Laboratories, and its support is gratefully acknowledged.

Title: Particle Blast Method (PBM) for the Simulation of Blast Loading

Author(s): Hailong Teng, *Livermore Software Tech. Corp.*.

This paper presents a particle blast method (PBM) to describe blast loading. The PBM is an extension of corpuscular method (CPM), which is coarse-grained multi-scale method developed for ideal gas dynamics simulation. It is based on the kinetic molecular theory, where molecules are viewed as rigid particles obeying Newton's laws of mechanics, while each particle in the particle method represents a group of gas molecules. Pressure loading on structures is represented by particle-structure elastic collisions. The particle blast method could be coupled with discrete element method, make it possible to model the interaction among high explosive detonation products, the surrounding air, sands and structure.

Title: Implementation of Non-Linear Finite Volume Discretization Methods in AD-GPRS

Author(s): Kirill Terekhov, Hamdi Tchelepi, *Stanford U.*; Bradley Mallison, *Chevron*.

This work covers implementation of several types of nonlinear finite-volume schemes with automatic differentiation capabilities of AD-GPRS. Nonlinear schemes correctly approximate fluxes on general polyhedral grids with full permeability tensor and preserve either positivity of the solution or discrete maximum principle. Convergence issues with the schemes preserving discrete maximum principle are discussed and a new improved formulation with flux decomposition into normal and transversal components is proposed. Nonlinear schemes are compared with multi-point flux approximations of type O, L and G on different black-oil problems.

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Title: Analysis Suitable Geometry

Author(s): Kevin Tew, Emily Evans, Michael Scott, *Brigham Young U.*; Guillermo Lorenzo Gomez, *U. A Coruna*; Derek Thomas, *UT Austin*.

In this talk we present our efforts to develop highly optimized data structures for analysis-suitable geometry representations like AST-splines and spline forests. These optimized geometry representations include the ability to perform localized h, p, and k adaptivity. Our optimized adaptivity and geometry operations enable isogeometric analysis to solve locally adapted 3D phase fields problems. Finally, we present new insights gained from designing algorithms for unstructured meshes.

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Title: Adaptively Weighted Numerical Integration in the Finite Cell Method

Author(s): Vaidyanathan Thiagarajan, Vadim Shapiro, *U. Wisconsin-Madison.*

With Adaptively Weighted (AW) numerical integration, for a given set of quadrature nodes, order and domain of integration, the quadrature weights are obtained by solving a system of suitable moment fitting equations in least square sense. The moments in the moment equations are approximated over a simplified domain that is homeomorphic to the original domain, and then are corrected for the deviation from the original domain using shape sensitivity analysis. In this talk, we will demonstrate the application of AW integration scheme in the context of the Finite Cell Method which must perform numerical integration over arbitrary domains without meshing. Traditional approaches to integration rely on fictitious domains, discontinuous functions, and/or adaptive subdivision. By contrast, in AW scheme the quadrature weights directly adapt to the complex geometric domain. We will demonstrate the computational efficiency of AW over traditional adaptive integration schemes as it requires fewer subdivisions and lesser time to achieve a given accuracy.

Title: Applications and Extensions of Bézier Projection Including Isogeometric Petrov-Galerkin Methods

Author(s): Derek C. Thomas, Thomas J. R. Hughes, *UT Austin*; Michael A. Scott, *Brigham Young U.*

The analysis of both B-splines and T-splines has benefitted from the introduction of spline dual functionals that are defined in terms of functions that are biorthogonal to the spline basis functions [1, 2]. However, numerical analysis based on splines has not yet benefited significantly from dual functionals although preliminary investigations have been performed [3, 4]. Potential applications include methods with diagonal mass matrices for the analysis of dynamical systems [3], isogeometric mortar methods [4], and the construction of weakly conforming geometries for isogeometric analysis. We present methods for construction of spline-biorthogonal functions in forms that are suitable for integration in element-based isogeometric analysis and draw connections to the recently introduced technique of Bézier projection [5]. We consider the relative performance of these biorthogonal functions in projection problems and in isogeometric Petrov-Galerkin methods. The use of biorthogonal functions in Petrov-Galerkin techniques is especially promising as it provides a consistent method to obtain higher-order lumped mass methods for explicit dynamics. REFERENCES [1] L. L. Schumaker, Spline functions: Basic theory, 3rd Edition, 2007, Cambridge University Press [2] L. Beirão da Veiga, A. Buffa, D. Cho, G. Sangalli, Analysis-suitable T-splines are dual-compatible, Computer Methods in Applied Mechanics and Engineering, Volumes 249–252, 1 December 2012, Pages 42-51 [3] J.A. Cottrell, T.J.R. Hughes, Y. Bazilevs, Isogeometric analysis: Toward integration of CAD and FEA, 2009, John Wiley & Sons, Ltd [4] E. Brivadis, A. Buffa, B. Wohlmuth, L. Wunderlich, Isogeometric mortar methods, Computer Methods in Applied Mechanics and Engineering, Volume 284, 1 February 2015, Pages 292-319 [5] D.C. Thomas, M.A. Scott, J.A. Evans, K. Tew, E.J. Evans, Bézier projection: A unified approach for local projection and quadrature-free refinement and coarsening of NURBS and T-splines with particular application to isogeometric design and analysis, Computer Methods in Applied Mechanics and Engineering, Volume 284, 1 February 2015, Pages 55-105

Title: Fluid-Structure Coupling Methods for Blast Loading on Thin Shells

Author(s): Jesse Thomas, Edward Love, Kevin Ruggirello, Martin Heinstein, William Rider, *Sandia Nat'l. Lab.*

Computational simulation of structures subjected to blast loadings requires the combination of blast shock-physics and structural response. Current methodologies, particularly for thin-shell structures, are problematic in terms of efficiency and solution quality. Algorithms that couple these physics should adhere to conservation principles and accept disparate discretizations. We present a high-fidelity, conservative, fluid and thin-shell-structure Fluid Structure Interaction (FSI) capability that uses finite volume shock physics methods, level sets, and unstructured shell modeling. We provide a two-field representation of the coupled FSI problem that uses constraints to tie the Lagrangian shell mesh to a level set embedded within the structured shock physics grid. Much of our focus is on the formulation and solution of this domain-to-domain coupling problem to produce high fidelity boundary conditions. We use adaptive approximations that do not anomalously transfer information across boundaries (being effectively one sided), thus reducing spurious oscillatory side effects in the coupling. The level set technique is widely employed to embed a solid boundary in a fluid flow (Cirak et al. 2007; Legay et al. 2006; Wang et al. 2011) and naturally provides detailed coupling regarding the geometry of the Lagrangian thin shell mesh. The literature presents a wide range of sophistication in coupling algorithms for interface enforcement. Simple but extremely flexible velocity and pressure transfer algorithms are available (e.g. Cirak et al. 2007), which include loosely coupled independent solvers. Many sophisticated but more specific algorithms are also available (e.g. Legay et al. 2006; Wang et al. 2011). We explore the influence of boundary representation techniques and coupling algorithms on the accuracy and convergence rates of our FSI problems. The tradeoffs of accuracy, convergence, and algorithmic efficiency are a key result of this work. F. Cirak, R. Deiterding, S.P. Mauch. Large-scale fluid-structure interaction simulation of viscoplastic and fracturing thin-shells subjected to shocks and detonations. *Comp. & Struct.*, 85, 2007, pp. 1049-1065. A. Legay, J. Chessa, T. Belytschko. An Eulerian-Lagrangian method for fluid-structure interaction based on level set. *Comp. Meth. App. Mech. Eng.*, 195, 2006, pp. 2070-2087. K. Wang, A. Rallu, J.-F. Gerbeau, C. Farhat. Algorithms for interface treatment and load computation in embedded boundary methods for fluid and fluid-structure interaction problems. *Int. J. Num. Meth. Fluids*, 67, 2011, pp. 1175-1206. 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.

Title: Graph-Based Adaptive Insertion of Cohesive Elements on Non-Simplicial Meshes

Author(s): James Thunes, Spandan Maiti, *U. Pittsburgh*; Alejandro Mota, James Foulk, *Sandia Nat'l. Lab.*.

Fracture and failure phenomena are of particular interest in the computational mechanics community. Historically, these subjects are studied using either Cohesive Element (CE) or eXtended Finite Element Methods (XFEM). In the CE method, a cohesive surface (an initially zero-thickness surface element which grows under loading) is introduced at the boundaries of the volumetric finite elements. Traditionally, these elements are added a priori. This method is computationally efficient, but is limited by knowledge of the problem. If the failure behavior is known, CEs can be inserted along the preferred crack path. If however the behavior is not known, a priori methods must insert CEs along all potential crack paths – expensive at run time due to the large number of unused crack paths. For this reason, adaptive methods have been developed which insert the CEs during the course of the simulation based on the stress state in the body. Unfortunately, adaptive insertion requires update of the finite element mesh during the course of the analysis. As a problem may require thousands of cohesive element insertions over the course of the simulation, an adaptive insertion algorithm that is robust and computationally efficient is required. A recent paper by Mota, et al.[1] has proposed an adaptive insertion method based on computational topology. In this method, the finite element mesh is represented as a mathematical graph. The topological elements of the finite element mesh (the nodes, edges, faces, and volumes) are represented as graph nodes while the edges of the graph represent the connectivity information of the mesh. All insertions are based on a small number of repeatable graph update rules that negate the need for many special cases for degenerate cases. However, this method was formulated for simplicial (i.e. triangle and tetrahedral) meshes. We show that this method can be generalized to nonsimplicial (e.g. hexahedral element) meshes. Time complexity of the method is the same as for the simplicial mesh algorithm from Mota, et al. The performance of the method is demonstrated with several examples. [1] A. Mota, J. Knap, and M. Ortiz, “Fracture and fragmentation of simplicial finite element meshes using graphs,” *Int. J. Numer. Methods Eng.*, vol. 73, no. 11, pp. 1547–1570, 2008.

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Title: Local Limits and Asymptotically Compatible Discretization of Nonlocal Elastic Models

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

In recent works of Tian-Du, a variational framework has been established to connect the approximations of linear nonlocal models (such as linear bond and state-based peridynamic equations) with that of linear elasticity. We present the extension to nonlinear problems that are technically much more challenging to analyze. The new results are particularly applicable to cases where the nonlocal elastic energy may not be convex.

Title: Cyclic Plastic Hinges with Degradation of Stiffness and Strength

Author(s): Lasse Tidemann, Steen Krenk, *Techn'l. U. Denmark* .

Elasto-plastic frame structures exposed to cyclic loads larger than the elastic limit load will develop cyclic yielding in concentrated zones acting as yield hinges. The yield hinges develop at the most severely loaded sections and are associated with the largest deformations in the structure. The formation of yield hinges typically lead to redistribution of the internal forces and may lead to degradation of the stiffness and strength of the structure and eventually failure of the structure. A fairly simple but versatile cyclic plasticity model with degradation effects has recently been developed [1]. It is here extended from the original stress-based format to a format based on the section forces in a beam cross section. The developed model includes simple, physically observable parameters for each component included in the yield surface; two stiffness parameters, initial yield capacity, ultimate capacity and a parameter describing the stress range between the yield capacity and the ultimate capacity. A 3D beam element is formulated in an equilibrium format from which the elastic stiffness matrix as well as the elasto-plastic stiffness matrix can be derived directly without the need for numerical integration over the cross section or the length of the beam. The determination of the elasto-plastic stiffness matrix includes a simple inversion of a matrix of size 2 by 2. The matrix inversion is dependent on the gradient of the yield surface which typically includes corners with an undefined gradient. To avoid this problem, a composite smooth, generic yield surface concept has been developed and applied with great accuracy to the yield surface of a tubular beam. Degradation of the model parameters is introduced in a way analogous to classical damage mechanics. Typical degradation mechanisms in low-cycle fatigue of tubular structures include local buckling, weld fracture, and punching shear [2,3]. In spite of the simple form of the present degradation formulation, the representation of observed cyclic degradation is rather good, even when compared to more complex models [2,3].

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Title: Finite Element Modeling and Validation of Thermal-Mechanical Behavior of Additive Manufacturing of Ti-6Al-4V

Author(s): Albert To, Qingcheng Yang, *U. Pittsburgh.*

Additive metal deposition processes using laser or electron beam heat sources are becoming increasingly popular due to their potential of manufacturing near net shape structural components. The thermal response in the deposition process is essential with respect to determining the resulting thermal and mechanical properties of the deposit materials. In this work, a 3D finite element model is developed and validated for predicting the thermo-mechanical behavior of Ti-6Al-4V during a laser engineered net shaping (LENS) process. The double ellipsoid volumetric heat source mode proposed in [1] is employed as the heat input model. The thermal problem is solved with hexahedral element using the element activation/deactivation technique. The mechanical problem is solved by employing a thermo-elastic-plastic constitutive model in which the material parameters are calibrated based on the tensile test experiments at different temperature and strain rates with the printed Ti-6Al-4V samples. Temperature and deformation measurements are performed in order to validate the simulation model. It is shown that the computed thermal history and mechanical deformations are in reasonable agreement with the experimental measurements. [1] J. Goldak, A. Chakravarti, M. Bibby, A new finite element model for welding heat sources, *Metallurgical Transactions B*, 15B(1984) 299-305 [2] A. Lundback, L.E. Lindgren, Modelling of metal deposition, *Finite Elements in Analysis and Design*, 47 (2011) 1169-1177 [3] J. C. Heigel, P. Michaleris, E.W. Reutzel, Thermo-mechanical model development and validation of directed energy deposition additive manufacturing of Ti-6Al-4V, *Additive Manufacturing*, 2015

Title: Understanding Grain Boundary Embrittlement and its Correlation with Polycrystalline Tungsten Fracture

Author(s): Hongsuk Lee, Vikas Tomar, *Purdue U. W. Lafayette.*

Grain boundary (GB) embrittlement has been repeatedly reported in fracture of refractory metals. It is suggested that the GB embrittlement is due to ductility loss by material addition and its segregation. While there are a few hypotheses available, one of the guiding explanations is that mechanism of GB embrittlement by segregation is from creation of a barrier to dislocation propagation by formation of a hardened region near the boundary. In case of tungsten (W) – nickel (Ni) alloy, ductility loss by Ni addition is known to be not related to the change of grain size, however, geometry of GBs is found to have high dependence with the GB embrittlement as well as material properties of W. GBs in W-Ni alloy are found to have thickness as a function of the level of saturation of W atoms with respect to Ni atoms in the GBs. The present work focuses on both atomic scale and continuum scale. The study in atomic scale examines (110)-(210) W GB mechanical strength as a function of thickness using an ab initio calculation framework based on Car-Parrinello molecular dynamics (CPMD) simulations. The atomic fraction of Ni atoms is varied to understand the influence of an addition and its correlation with thickness variation on the GB fracture strength. Based on the analyses performed, an analytical relation to predict GB peak tensile strength as a function of atomic cohesive energy, GB thickness (level of saturation), and the Ni atomic fraction is proposed. Then extended finite element method (XFEM) simulations have been conducted in continuum scale, with applying obtained GB peak tensile strength in atomic scale, to derive GB embrittlement in quantitative expression by introducing revised brittleness index, which takes account of length-scale effect.

Title: Closure Models for High-Order Finite Element Hydrodynamics

Author(s): Vladimir Tomov, LLNL.

In this talk we present our approach in developing a multi-material extension of the high-order finite element Lagrangian method described in [1]. Lagrangian codes solve the hydrodynamics equations on a moving mesh. In order to compute correct pressure, such algorithms must be able to handle the so-called mixed cells where a single computational element contains multiple materials. Mixed cells appear when aligning the mesh to the material interfaces is not desirable, or the Lagrangian algorithm is combined with a remesh procedure. The goal of a closure model is to define evolution of material volumes, during a Lagrangian simulation, in a physically reasonable way. We re-formulate some of the existing methods (e.g. [2]) for the low-order, cell-centered case, as multi-material mathematical models on a continuous level, thus extracting and separating the model from the discrete algorithm. Then we apply a high-order finite element discretization to this continuous model. This combination results in a pressure equilibration procedure that defines terms which control the evolution of material volume and the transfer of internal energy between distinct materials. These terms are computed at each integration point of a mixed cell, complying with the high-order finite element concept of sub-cell resolution without the need of reconstructing an explicit material interface. Using the single-material discretization in [1] as a base, we duplicate the material density and energy for every material present in a zone, but use a single velocity, motivated by the fact that the conforming computational mesh has a single motion during a Lagrangian computation. In addition, a set of new variables, i.e. volume fractions, is added to the zonal data that describes the distribution of the materials within the zone. These volume fractions can be represented as pointwise values at a chosen set of integration points on a reference cell, or arbitrarily high-order finite element functions. This spatial discretization is combined with high-order explicit time stepping methods. We will show the details of the above discretization and illustrate the numerical performance of the resulting algorithms on a set of model multi-material test problems. References: [1] V. Dobrev, Tz. Kolev, and R. Rieben, High order curvilinear finite element methods for Lagrangian hydrodynamics. *SIAM J. Sci. Comp.*, 5(34):B606–B641, 2012. [2] M. Shashkov, Closure models for multimaterial cells in arbitrary Lagrangian-Eulerian hydrocodes, *Int. J. Numer. Meth. Fluids* 56:1497–1504, 2007.

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Title: Formulation and Implementation of the 3D Shallow Water Adaptive Hydraulics (AdH) Software

Author(s): Corey Trahan, *ITL, ERDC, USACE*.

The Adaptive Hydraulics (AdH) software suite is a state-of-the-art modeling system developed by the Coastal and Hydraulics and Information Technology Laboratories, ERDC, USACE. AdH is a multi-physics, implicit finite element suite, focused on both 2d and 3d shallow water models. Some features of AdH include: adaptive mesh control, time-adaption, shallow water 2d wetting and drying, general transport and cohesive/noncohesive sediment transport via the sediment library SEDLIB. Particular focus of this talk will be on the newly added AdH 3d shallow water, baroclinic model. The 3d shallow water model formulation and implementation will be summarized, and recent HPC applications of the model on Mobile and Galveston Bay will be presented. Also discussed will be the 3d shallow water linkage to SEDLIB, an ERDC sediment transport library.

Title: Automated Tuning for Parameter Identification in Multi-Scale Coronary Simulations

Author(s): Justin Tran, Daniele Schiavazzi, Abhay Ramachandra, Andrew Kahn, Alison Marsden, *UC San Diego*.

Computational simulations of coronary artery flow can provide non-invasive information on hemodynamics and wall mechanics that can aid in treatment planning and improve understanding of disease mechanisms. Examples of clinical applications include identifying optimal geometries for coronary artery bypass grafts, determining risk of stenosis on saphenous vein grafts, and determining thrombotic risk in Kawasaki disease. In this study, patient-specific geometries are constructed from CT scans and combined with finite element flow simulations using the open source software package SimVascular (simvascular.org). Lumped parameter networks (LPN), consisting of 0D circuit element representations of hemodynamic behavior, are used to represent the heart and distal circulation that are not included in the 3D model. These networks provide a set of ODEs that can be solved for global hemodynamic quantities and used as coupled boundary conditions for the finite element flow solver [1]. The parameters of the LPN (e.g. vessel resistance, compliance, inductance, etc.) are typically tuned so the outputs match a patient's clinical data. However, the myriad parameters in these systems are usually subject to manual tuning which is time consuming and produces operator-specific parameter values that do not account for the uncertainty in the clinical measurements. This laborious process also makes application to large clinical cohorts challenging. We thus propose a Bayesian registration framework combining preliminary local sensitivity analysis with adaptive Markov Chain Monte Carlo sampling. LPN models simulating coronary flow are characterized by a large number of parameters and relatively scarce available clinical data. The data we use to estimate the parameter values of the LPN consist of patient-specific echocardiography data, clinical data, and literature data on Doppler flow wire measurements in the coronaries [2]. We have 35 parameters and 22 targets in our coronary LPN models, resulting in overparameterization. After an extensive review of the literature and data available from echocardiography for coronary physiology, collection of additional targets appears unlikely. We therefore focus efforts on parameter reduction. Preliminary parameter reduction has been done using the Fisher information matrix to determine parameters which do not make a significant impact on our clinical targets of interest. This will be expanded by analyzing the samples resulting from MCMC, leading to improved understanding of which parameters are strongly correlated or poorly estimated. [1] Sankaran, S et al., *Annals of Biomedical Engineering*, 20:2228-2242, 2012. [2] Ofili, E et al, *American Journal of Cardiology*, 71.14:D3-D9, 1993.

Title: Large Eddy Simulation Based on Residual-Based Variational Multiscale Formulation and Lagrangian Dynamic Smagorinsky Model

Author(s): Steven Tran, Onkar Sahni, *RPI*.

One of the challenges in modeling turbulent flows is the multi-scale nature of turbulence. For many practical applications, the Reynolds number is sufficiently high that the cost of directly simulating turbulent flows is prohibitively high. On the other hand, models such as those used in Reynolds-averaged Navier Stokes (RANS) simulations fail to capture accurately much of the unsteady dynamics of turbulent flows. However, large eddy simulation (LES) provides greater fidelity in which the large-scale flow structures are resolved while their interactions with the subgrid scales are modeled. One commonly used LES model is the Smagorinsky model where filtering is done to model the unresolved stresses. The unresolved stresses are based on an eddy viscosity model which in-turn involves the Smagorinsky constant that may vary in space and time depending on the problem. While dynamic procedures exist for approximating this constant, it has been shown to be numerically unstable unless averaging is applied. Spatial averaging is typically applied across homogeneous directions however this limits the problems that can be studied. On the other hand, Meneveau et al. [1] proposed Lagrangian averaging over fluid pathlines for complex turbulent flows with inhomogeneity. In contrast to the Smagorinsky model, the residual-based variational multiscale (RBVMS) formulation [2] has also been recently developed for LES. Moreover, a mixed model has been developed and applied in [3], where RBVMS was used to model the cross-stress terms while dynamic Smagorinsky model based on averaging over homogenous directions was employed for the Reynolds stress terms. In this work, we will focus on the combinations of the residual-based variational multiscale formulation and the Lagrangian dynamic Smagorinsky model in order to perform LES of turbulent flows with inhomogeneity. We will also present the effects of different filtering schemes including both 2D and 3D filtering schemes. Applications will range from turbulent channel flow to flow over an airfoil. Comparisons with DNS and/or experimental data will be made. References: [1] Meneveau, C., et al. "A Lagrangian dynamic subgrid-scale model of turbulence." *Journal of Fluid Mechanics* 319 (1996) [2] Bazilevs, Y., et al. "Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows." *Computer Methods in Applied Mechanics and Engineering* 197.1 (2007) [3] Wang, Z., et al. "A mixed large eddy simulation model based on the residual-based variational multiscale formulation." *Physics of Fluids* (1994-present) 22.7 (2010)

Title: T-Stress Calculation for Cracks in 2D Anisotropic Elastic Media

Author(s): Han Tran, *Vietnamese-German U.*

A numerical procedure is proposed to compute the elastic T-stress for two-dimensional cracks in general anisotropic elastic media. T-stress is obtained from the sum of crack-face displacements which are computed via a regularized integral equation of the boundary data. To avoid taking a numerical differentiation, an integral equation for the derivative of crack-face displacements with respect to the arc length of crack is formed in a weak sense so that this quantity can be obtained directly at the crack tip as the solution of a system of equations for nodal values. The procedure is incorporated in a symmetric Galerkin boundary element method (SGBEM) in which all the integral equations for the data (i.e. traction and displacement) on boundaries and crack surfaces contain only weakly-singular kernels of order $\ln r$. Numerical examples for cracks in unbounded and finite domains are treated and it is shown that highly accurate results are obtained using the proposed method.

Title: Stochastic Analysis of Mesoscopic Elasticity Random Fields Obtained by Filtering Framework

Author(s): Vinh Tran, Sebastien Brisard, Karam Sab, *Lab. Navier - ENPC*; Johann Guilleminot, *Lab. MSME - U. Paris Est*.

Periodic homogenization of random heterogeneous materials generally requires the description of a complex, underlying random microstructure. In this context, Bignonnet et al. recently proposed a framework where smooth mesoscopic elasticity random fields are defined through a filtering procedure [1], hence allowing for the use of coarser discretizations in numerical homogenization methods. Interestingly, the above random fields have the remarkable consistency property to yield the same effective moduli at macroscale, regardless of the filtering resolution. The present work is devoted to the construction, calibration and validation of a prior elasticity random field representation for a model microstructure. For illustration purposes, the latter is made up of an elastic matrix reinforced by bi-disperse spherical stiff heterogeneities. On the basis of a statistical characterization, we first discuss the use of an information-theoretic model along the lines derived in [2]. Next, the calibration task is performed by using either statistical estimators or the maximum likelihood principle. Both approaches are compared in terms of convergence and computational cost. Finally, the validation of the model is discussed by comparing some quantities of interest (such as the induced mesoscale stress field or the macroscopic homogenized properties) that are obtained either from numerical experiments on the underlying random microstructure or from model-based simulations. References: [1] F. Bignonnet, K. Sab, L. Dormieux, S. Brisard, and A. Bisson. Macroscopically consistent non-local modeling of heterogeneous media. *Comput. Method. Appl. M.*, 278:218–238, 2014. [2] J. Guilleminot and C. Soize. Stochastic model and generator for random fields with symmetry properties: Application to the mesoscopic modeling of elastic random media. *Multiscale Model. Sim.*, 11(3):840–870, 2013.

Title: Modeling Delamination in Composites Under Dynamic Loading Using a Stabilized Discontinuous Galerkin Approach

Author(s): Timothy Truster, Wesley Hicks, *U. Tennessee, Knoxville.*

This paper presents a consistent numerical framework for modeling delamination in fibrous composites under dynamic loading. Under extreme loading such as impact, the interfaces or junctures between the constituent materials of the fiber-matrix composite can be the sites of stress concentrations that lead to fracture and weakening of the structural component. Therefore, accurate simulation of such composite structures is important for predicting the remaining structural life span and whether the component remains fit for service. The traditional technique for modeling debonding is the embedding of traction-separation laws into interface elements in the finite element model, leading to so-called intrinsic cohesive zone models (CZM). However, this approach faces key issues in the dynamic context due to the artificial compliance induced by the initial interface stiffness required in the elements prior to debonding initiation. Selecting the value for the artificial stiffness requires a great deal of calibration to ensure both that the elastic wave speed of the undamaged specimen is unaltered and that the critical time step for explicit dynamics does not become vanishingly small. As an alternative, we present a stabilized Discontinuous Galerkin (DG) method for modeling the evolution of damage at interfaces using both implicit and explicit time integration schemes. The key idea is the incorporation of a debonding or damage variable at the Gauss points along the interface representing the inelastic gap or separation, similar to the treatment of the plastic strain field in the context of computational inelasticity. The condition that the jump in the finite element displacement field at the interface is equal to this debonding field is weakly enforced using the DG method. Initially when damage is not present, the displacement field between the fiber and matrix are weakly continuous, thereby removing the issue of artificial compliance. After a yield/fracture criterion is exceeded, the inelastic gap is evolved through constitutive relations as a function of the interface traction computed from the numerical flux terms. By utilizing analytical expressions for the penalty parameter [1], the calibration of the computational model involves only the selection of physical parameters in the constitutive interface model. Numerical results for a variety of benchmark problems involving dynamic delamination confirm the robustness of the method. [1] Truster T.J., Masud A. (2013). Primal interface formulation for coupling multiple PDE: A consistent derivation through the variational multiscale method. *Computer Methods in Applied Mechanics and Engineering*, 268:194-224.

Title: Optimal Bayesian Experimental Design for Contaminant Transport Under Uncertainty

Author(s): Panagiotis Tsilifis, Roger Ghanem, *U. Southern Cali.*

Experimental design is of crucial importance for inference where limitations in the data collection procedure are present due to cost or other restrictions. Optimal experimental designs determine parameters that in some appropriate sense make the data the most informative possible. In a Bayesian setting this is translated to updating to the "best" possible posterior. Information theoretic arguments have led to the formation of the expected information gain as a design criterion. This can be evaluated mainly by Monte Carlo methods and be maximized by using stochastic approximation methods, both known for being computationally expensive tasks. We propose an alternative framework where a lower bound of the expected information gain is used as the design criterion that helps decrease the computational burden involved in the above mentioned steps as well as eliminates the induced bias. The problem of permeability inference in a large contaminated area is used to demonstrate the validity of our approach where we use the massively parallel version of the multiphase multicomponent simulator TOUGH2 to simulate contaminant transport and a Polynomial Chaos approximation of the forward model that further accelerates the objective function evaluations.

Title: Multi-Scale Crystal Defect Dynamics (MCCD): A Quasi-Crystal Model for Defect Dynamics

Author(s): Qinson Tu, Shaofan Li, *UC Berkeley*.

Recently the author and his co-workers have developed an atomistic based multiscale crystal defect dynamics (MCDD), which is based on a postulate that each ideal crystal lattice is associated with a quasi-crystal lattice which is the inherent microstructure of defects in that ideal crystal. In this approach, we can model defects by modeling the corresponding quasi-crystal, which is characterized by the so-called lattice process zone. All the nonlinear deformation is assumed to be confined inside the process zones. Coarse grain models are adopted for both the bulk medium and crystal process zone. In bulk elements the first order Cauchy-Born rule is used to model its material constitutive behaviors, and in all crystal process zones, higher order Cauchy-Born models are used to model their constitutive relations, so that we can formulate an atomistic enriched continuum constitutive relation to describe the whole crystalline material behaviors. Since Inside the interphase zone, the higher order Cauchy-Born rules are adopted in process zones, and a hierarchical higher order strain gradient coarse grain constitutive model is derived, which can capture the size-effect at the small scales. All interphase or process zones are constructed such that they are part (a subset) of slip planes in a lattice space. The multiscale crystal defect dynamics has been applied to simulate both dislocation motion and crack propagations in both single crystals and poly-crystals. We have defined and discovered a so-called element mesh stacking fault energy, whose behaviors will result different slip motions and fracture patterns for both brittle as well as ductile behaviors. Crack branching and void formation have been found possible for different element mesh stacking fault energies, which are dictated, by the effective lattice structure or microstructure in the process zone elements.

Title: Algebraic Multigrid Preconditioners for Q2-Q1 Discretizations of the Incompressible Navier-Stokes Equations

Author(s): Ray Tuminaro, *Sandia Nat'l. Lab.*

Algebraic multigrid (AMG) preconditioners are well established for PDE systems where all unknown types (e.g., pressures and velocities) are co-located at mesh points. In this situation, unknown types are coarsened in a fashion such that they remain co-located at coarse mesh points throughout a multigrid hierarchy. In this talk, we consider AMG preconditioners for complex discretization schemes where unknowns are not necessarily co-located. Specifically, we investigate a Q2-Q1 mixed finite element discretization of the incompressible Navier-Stokes equations as well as a potential formulation of a resistive magnetohydrodynamics (MHD) system. For Q2-Q1 discretizations, the relationship between velocity and pressure spaces is carefully chosen to satisfy a discrete inf-sup condition and guarantee the stability of the fine grid discretization. In developing a multigrid method, it would be desirable to also guarantee the stability of coarse level operators. Unfortunately, this is not possible with a straightforward application of a black-box AMG library, as no special consideration is given to the Q2-Q1 structure. In this talk, we describe a new energy minimization AMG (EMIN-AMG) preconditioner that mimics certain pressure/velocity relationships of a Q2-Q1 discretization on coarse grids. The basic idea is to first automatically define coarse pressures (in a usual algebraic multigrid way) and then to carefully choose the coarse velocity unknowns such that they are consistent with the coarse pressures. A key theme underscoring the new algorithm is that of leveraging flexibility inherent in an EMIN-AMG scheme to develop the consistent coarse spaces. Numerical results highlighting the performance of the new solver will be given on a number of incompressible problems including an MHD example application. For the MHD example, we use a family of new multigrid smoothers that correspond to extensions of commonly used smoothers for incompressible flow (Vanka smoothing and Braess-Sarazin smoothing).

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Title: Towards Digital Image Correlation Methods Robust Enough to Characterize Degradation of Materials

Author(s): Daniel Turner, *Sandia Nat'l. Lab.*

Clearly, the strong resurgence of digital image correlation (DIC) as a non-contact means of obtaining full-field displacements speaks to its efficacy and usefulness. Still, there remain a number of limitations in the mathematical formulation of the basic DIC process that prevent its application to some challenging, but important problems of interest. In particular, problems that involve characterizing damage or degradation of materials, as these inherently involve steep strain gradients and discontinuities in the displacement field. Current DIC methods require a tremendous amount of interventions or ad-hoc modifications to be applied to these types of problems. As an alternative approach, we propose developing a DIC method using nonlocal operators rather than classical spatial derivatives. In this way we expand the space of displacement fields appropriate for DIC to include discontinuous and non-differentiable fields in a mathematically consistent fashion without the need for sophisticated algorithmic modifications. This talk will provide the mathematical context for nonlocal image correlation and show how it ties into nonlocal mechanics (for example, peridynamics).

Title: Simulating the Effects of Compaction, Pore-Plugging, and Grain-Crushing on the Permeability and Beta Factor of Porous Media Using Lattice Boltzmann Method

Author(s): Mayank Tyagi, Sultan Anbar, *LSU*; Ali Takbiri-Borujeni, *WVU*.

Near wellbore flow phenomena during high rate production or injection of fluids can include a variety of physical processes that alter the macroscopic media properties such as permeability and beta factor (Forchheimer or non-Darcy coefficient). In particular, the pressure losses induced due to the flow inertia at high rates is not well understood under the conditions of compaction, pore plugging or proppant crushing. In this study, lattice Boltzmann method (LBM) based simulations are used to calculate the changes in media properties by resolving the flow in the pore-spaces of either idealized porous medium (sphere-pack) or image-based porous media. LBM also exploits the recent advances in the high performance computing (HPC) capabilities and thus, resolves the flow details in representative elemental volumes (REV) by using large meshes inside the pore-spaces of media to capture the topology of pore connections. A wide range of physical processes are modeled using varied pore-space representations by modifying the grain shapes and packing for compaction, deleting pore throat connections for pore-plugging, and using X-ray images of proppant packs under different stress conditions. Calculated permeability and beta-factor for various particle size based Reynolds number are analyzed to understand the behavior of macroscopic porous media properties at high flow rates that are expected in the near wellbore region. A few representative results from simplified near wellbore region reservoir simulations are presented here that incorporated the newly developed correlations for permeability and beta-factors from pore-scale simulations. Significant impacts on well productivity indices are shown while accounting for the changes in permeability and beta factors to represent compaction, pore-plugging, and grain crushing in the near wellbore region of the reservoirs. References: 1. Takbiri-Borujeni, A., Multi-scale Modeling of Inertial Flows through Propped Fractures, Ph.D. dissertation, Louisiana State University, Baton Rouge, 2013. 2. Anbar, S., Multi-scale Estimation of Inertial Effects for Frac-pack Completed Gas Reservoirs, Ph.D. dissertation, Louisiana State University, Baton Rouge, 2014.

Title: Residual-Based Stabilized Formulations for the Solution of Inverse Elliptic PDEs

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

We consider an inverse problem associated with elliptical partial differential equation. The typical problem includes determining thermal conductivity for a system from temperature measurements, or determining shear modulus from displacement measurement. We take homogeneous elliptical partial differential equation governing the system, where we seek to determine material properties from measured response. This problem can be posed as a minimization problem where we try to minimize the difference between the predicted and the measured response in L_2 norm, where the predicted response is constrained to satisfy the governing partial differential equation (pde). This is achieved by constructing a Lagrangian, where the pde is enforced through the Lagrange multiplier. To solve the inverse problem, we setup the first variations of the Lagrangian to zero to obtain a saddle point problem. The Galerkin formulation of the linearized saddle point problem yields a saddle point system of equations. The LBB conditions applied to this system shows that the problem lacks stability [1]. As, an alternative, instead of the LBB conditions, we can look at the inf-sup condition for the whole saddle point system, which, in spite of being a weaker condition than coercivity, is sufficient for optimal discrete solution. The inf-sup condition for the whole system shows that there is an added stability to the problem, however it is not sufficient. To overcome the remaining lack of stability, we add a residual based stabilization term to the Galerkin formulation. To prove convergence of the stabilized formulation, we use Nitsche's trick [2], which comprises of suitably defined adjoint problem, inverse estimates, and regularity estimates. To prove effectiveness of the stabilized formulation, we consider a benchmark problem to show optimal convergence rate. References: [1] T.J.R Hughes, L.P.Franca, M. Balestra, A new finite element formulation for computational fluid dynamics: V. circumventing the Babuska-Brezzi condition: a stable Petrov-Galerkin formulation of the stokes problem accommodating equal-order interpolations, *Computer Methods in Applied Mechanics and Engineering* 59 (1986) 85-99. [2] Brenner, S., Scott, L. (1994). *N-Dimensional variational problems. In the mathematical theory of finite element methods* (pp. 135-140). Springer-Verlag.

Title: Finite Element Analysis of Adiabatic Flows

Author(s): Ichiro Uchiyama, *Ocean Consultant Japan Co.*; Mutsuto Kawahara, *Chuo U.*

Currently, a large number of fluid flow analysis using Navier - Stokes equation has been carried out by assuming incompressible condition. The reason of utilization of incompressible assumption is that the basic equations are limited to the conservation of mass and momentum and variables are velocity and pressure, and it is not required to solve the density changes. However, incompressible state is a limited state of compressibility, and slight changes in the density are existing in the actual flows. On the other hand, some of the adiabatic flow models have been developed by considering the slight changes in the density. It have been applied the SUPG method or the bubble function method for the flow in order to stabilize the analysis. These methods are widely used for fluid flow analysis by controlling the numerical viscosity, and are verified in a lot of cases. For the advantage of adiabatic flow model, the density is able to consider being a function of the pressure by neglecting the thermal changes in the fluid. Thus, this model does not need to solve the Poisson equations and the computational burden is expected to be low. In this study, first, to using explicit approach and Eulerian formulation, the applicability of the ideal the gas problem, which are the flows in the cavity and flows around a cylinder, is confirmed. Next, in the near future, aiming at the application of the structural design of marine structures, port and harbor facilities against wave action, the effectiveness of this model is confirmed in the solitary wave analysis. In case of solitary wave analysis, in order to consider the free surface changes, explicit approach and Lagrangian formulation are adopted.

Title: A Wave-Based Approach toward Precisely Controlled Dynamic Structural Demolition

Author(s): Koji Uenishi, *U. Tokyo*; Hiroshi Yamachi, *SMCON Co., Ltd.*

In order to actualize effective impact/blast-resistant design of structures, we must, first of all, understand the physical process behind the dynamic structural fragmentation, namely, dynamic wave propagation, interaction (reflection, diffraction, and so on) and development of fracture network in the structures considered. However, the details of dynamic fragmentation have not been fully clarified yet and the situation becomes challenging if the structure is complex. Here, as an initial step, we try to deepen our understanding of the mechanics of structural fragmentation by blasting (detonation of explosives [1]) or by electric discharge impulses (pulsed high-voltage electric discharge [2]). Also, by making use of the theory of wave dynamics, we wish to establish a more physics-based approach for designing efficient, precise and more quantitatively controllable dynamic fragmentation (demolition) of structures. Computationally, we utilize our fully three-dimensional finite difference code to acquire preferable geometrical and loading conditions for a given structure to be demolished. We compare the numerical results with the field observations of high-speed fracture experiments to validate our computations. As a result, for instance, we can indicate that geometrical settings of blast holes and empty dummy holes can truly control the dynamic wave propagation and crack development in structures and hence the final fragmentation patterns may be predicted in advance. Optimal positions of blast and dummy holes for demolition may be obtained for given structures by our numerical simulations, and the methodology developed in this study is useable for both conventional and modern dynamic fragmentation technologies, i.e. blasting and electric discharge impulses. References [1] Uenishi, K., H. Takahashi, H. Yamachi, and S. Sakurai (2010). PC-Based Simulations of Blasting Demolition of RC Structures. *Construction and Building Materials*, 24(12), 2401-2410. [2] Uenishi, K., H. Yamachi, K. Yamagami, and R. Sakamoto (2014). Dynamic Fragmentation of Concrete Using Electric Discharge Impulses. *Construction and Building Materials*, 67(B), 170-179.

Title: Combining 2-D and 3-D Image Segmentation Techniques Using Triangulated Surface Boolean Operations

Author(s): Adam Updegrove, Shawn Shadden, *UC Berkeley*, Nathan Wilson, *OSMSC*.

There are defined and recognizable processes for creating a complex 3-D patient-specific anatomic model. One can take a series of 2-D image segmentations and create a 3-D geometry through solid model lofting operations [1]. This has been used extensively for patient-specific blood flow simulation (e.g. [2]). It is also possible to use direct 3-D image segmentation techniques, which are widely popular and have been frequently utilized to construct localized anatomic models for clinically relevant problems such as cerebral and abdominal aortic aneurysms. The geometric extent of the anatomic models constructed directly from 3-D segmentation techniques, however, are often limited compared to anatomic models constructed from 2-D techniques due to factors including poor image quality and difficulty in selecting appropriate spatially-varying segmentation parameters in 3-space. Further, since 2-D segmentation techniques lead to the creation of boundary representation solid models (with vessel walls defined as NURBS) and 3-D techniques were simply spatial regions enclosed by a densely triangulated surface, it is difficult to combine models constructed using different segmentation techniques. This has led to a common accepted modeling tradeoff: more extensive and flexibly defined vascular models created by lofted 2-D segmentations, or less extensive and potentially better- conforming vascular models created by 3-D segmentation. In this work, a solution is proposed to enable the flexibility to combine both segmentation techniques for the creation of an optimal anatomic geometry: 3-D segmentation for certain regions of interest (e.g. aneurysmal sac) while simultaneously using lofted 2-D segmentations to include surrounding vasculature as desired. In particular, a technique to create triangulated vessels from 2-D segmentations without using solid modeling packages has been developed. This makes use of a new implementation of robust Boolean operations for complex triangulated surfaces that has been developed and implemented into the open source package SimVascular (www.simvascular.org). With these operations and customized geometric manipulation techniques, it is possible to leverage the advantages of 2-D and 3-D image segmentation techniques to create a quality anatomic geometry for blood flow simulation.

Title: Continuum Damage Model for Hydrogen Embrittlement in Ferritic Steels

Author(s): Dakshina Valiveti, Neeraj Thirumalai, *ExxonMobil*.

Hydrogen embrittlement of metals and alloys is a long standing technological challenge, and of great relevance to the oil and gas industry. The fundamental understanding of embrittlement mechanism(s) and the ability to model hydrogen embrittlement is important for managing the integrity of equipment. To that extent, the present work develops a mathematical model to estimate the strength degradation and model hydrogen embrittlement in steels. The proposed model adopts the Nano-Void Coalescence (NVC) theory [1] as the key damage mechanism. NVC is the most recent theory proposed in the literature for hydrogen embrittlement and provides a more robust micro-mechanical pathway to failure than previous models. A mathematical model is developed for hydrogen affected constitutive response of material, and solved within the framework of finite element method. The modified constitutive response is a Gurson plasticity based continuum damage model and incorporates key aspects of NVC failure theory. The deformation and damage in the material are coupled with trap mediated hydrogen diffusion [2]. Calibration of damage model parameters is performed for X65 commercial line pipe steel. The capability of the damage model is established with numerical simulation of failure in round bar tensile tests on X65 steel under hydrogen exposure. The numerical simulations are shown to be in excellent agreement with the experimental results. References: 1.T. Neeraj, R. Srinivasan, Ju Li, Hydrogen embrittlement of ferritic steels: Observations on deformation microstructure, nanoscale dimples and failure by nanovoiding, *Acta Materialia*, 2012, 60:5160–5171. 2.Dadfarnia M., Sofronis P., Neeraj T., Hydrogen interaction with multiple traps: Can it be used to mitigate embrittlement? *International Journal of Hydrogen Energy*, 2011, 36:10141–10148.

Title: Multi-Scale Modeling of Shale Gas, Study of Macroscopic Behavior and of Cracking Phenomenon

Author(s): Alexis Vallade, Jean-Baptiste Colliat, Jian Fu Shao, *U. Lille1*.

In the context of the exploitation of shale, gas reservoir rock is subjected to coupled hydromechanical stresses. To investigate the integrity of the well and the reservoir, and to improve operating techniques, it is necessary to carry out coupled numerical simulations taking into account failure. For low damage state, it is possible to assume that the cracks are isotropic and uniformly distributed. However, if the structure is heavily damaged, with one or more macro-cracks, the above hypothesis are no longer true. Here we choose to use a discrete cracking representation (through the E-FEM method) in order to carry out the computations for transfer. To represent a fine mineralogy in a large domain the number of degrees of freedom is high, in order to solve such a problem we must use the domain decomposition method. The model we present here is a model using a multi-scale analysis block type coupled with domain decomposition method (the mortar method). Using a kinematic enrichment of weak and strong discontinuities can be inserted within the same elements. These discontinuities can represent a heterogeneous medium (using low discontinuities) and a crack (strong discontinuities).

Title: Eigendeformations and Regularizations in Damage and Fracture Problems

Author(s): Nunziante Valoroso, Fernando Fraternali, Gabriele Cricri, *U. Napoli Parthenope*.

In the last two decades regularized formulations have become increasingly popular in Mechanics as techniques that allow dealing with problems suffering from mesh-sensitivity and time-stepping dependence induced by strain softening. In short, the idea underlying such techniques is that of using some extended constitutive equations in which information about the material microstructure is synthetically represented through a characteristic length scale parameter (i.e., in concrete this is believed to be about twice the average aggregate size). A complete damage state corresponds to the formation of a discrete fracture and a link between the two descriptions of material failure can be established following different approaches. For instance, successful implementations of the variational approach to fracture can be achieved in the form of a gradient-enhanced damage model [1] or introducing eigendeformations to develop displacement jumps [2]. In this communication common aspects to both approaches are discussed i.e., the fact that multi-field formulations are arrived at and also that models themselves are amenable to a physical interpretation not limited to a mathematical approximation of the parent fracture model, though the latter could be eventually recovered in the limit. Numerical examples of fracture and damage in solid bodies will be presented to show the effectiveness of the considered approaches. REFERENCES [1] Valoroso, N, 2015. Gradient enhancement for a damage model, to appear. [2] Schmidt, B, Fraternali, F, Ortiz, M, 2009. Eigenfracture: An Eigendeformation Approach to Variational Fracture. Multiscale Modelling and simulation, 7 (3); 1237-1266.

Title: Inversion Under Uncertainty Applied to Trace-Gas Transport

Author(s): Bart van Bloemen Waanders, Timothy Wildey, *Sandia Nat'l. Lab.*; Harriet Li, *MIT*.

The characterization of trace-gas sources is important to help control pollutants in the atmosphere. Carbon-dioxide is one of several species that has been linked to the increase of average global temperatures and understanding the overall dynamics of these trace-gases depends on reconstructing the spatial distribution and magnitudes of carbon-dioxide fluxes. This inversion is complicated by several factors: multiple spatial distributions, extreme sparsity of measurements, temporal variations, uncertainty of natural CO₂ sources and sinks, and the many uncertainties associated with data and model parameters. In particular, the velocity fields need to be calculated from complicated atmospheric models that exhibit considerable solution variability. In this work, we demonstrate an optimization approach that inverts for trace gas source terms and material properties using multi-species, convection-diffusion-reaction dynamics. A trust-region methodology with adjoint-based sensitivities and Newton-based algorithms are used to solve the inversion problem in which the constraints are discretized with Stabilized Upwind Petrov Galerkin (SUPG) finite elements. We investigate two critical aspects associated with this inversion. First an efficient inversion under uncertainty scheme is explored that leverages concepts from stochastic optimization. We solve for source terms and diffusivity parameters simultaneously while accounting for the stochastic velocity field by augmenting the objective function with an appropriate risk measure. The solution is deterministic but can be considered robust in the face of model uncertainty. Second, we enhance the information content of the data by considering measurements from multiple gas species. To avoid an inversion crime, our synthetically generated measurements are simulated on a higher fidelity grid and endowed with noise. Numerical results are presented that investigate the sensitivity of sensor sparsity, noise, and the number of sources. In addition, we investigate the sensitivity of adding measurements from other gas species to the quality of the solution. Our software implementation leverages several components from the Trilinos framework.

Title: Goal-Oriented Model Adaptivity for Viscous Flows

Author(s): Timo van Opstal, *Norwegian U. Sci. & Tech.*; Paul Bauman, *UT Austin*; Serge Prudhomme, *E. Polymtl*; Harald van Brummelen, *Eindhoven U. Tech.*.

In [1] airbag inflation simulations were performed where the flow was approximated by Stokes flow. Inside the intricately folded initial geometry the Stokes assumption is argued to hold. This linearity assumption leads to a boundary-integral representation, the key to bypassing mesh generation and remeshing. It therefore enables very large displacements with near-contact. However, such a coarse assumption cannot hold throughout the domain, where it breaks down one needs to revert to the original model. The present work formalizes this idea. A model adaptive approach is proposed, in which the surrogate model (a Stokes boundary-integral equation) is locally replaced by the original high-fidelity model (Navier-Stokes) based on a-posteriori estimates in the error in a quantity of interest. This adaptive modeling framework aims at taking away the burden and heuristics of manually partitioning the domain while providing new insight into the physics. We elucidate how challenges pertaining to model disparity can be addressed. Essentially, the solution in the interior of the surrogate model domain is reconstructed as a post-processing step. We furthermore present several steady, two-dimensional numerical experiments to show that the error estimator is reliable. References [1] T. Opstal, E. Brummelen, R. Borst, and M. Lewis. A finite-element/boundary-element method for large-displacement fluid-structure interaction. *Computational Mechanics*, 50(6):779–788, 2012.

Title: Towards Massively Parallel Higher-Order Immersed Domain and Isogeometric Finite Element Analysis

Author(s): Vasco Varduhn, Dominik Schillinger, *U. Minnesota*.

Recent high performance computing environments sum up to hundreds of thousands of cores and show an increasing level of heterogeneity. Such extensive computing power originates from multi-core CPUs and coprocessors such as GPGPU or Intel Xeon Phi. Modern parallel simulation environments must cope with largely varying transfer bandwidths between the processing units, multi-level cache hierarchies and varying latency. Significant additional challenges constitute the systematic implications of higher-order embedded and isogeometric finite element analysis. Immersed domain analysis based on the finite cell method uses higher-order non-boundary fitted meshes for the approximation of the solution fields. It eliminates cost-intensive mesh generation and transfers geometry handling to the adaptive integration of element matrices in intersected elements. As a result, the computational load of formation and assembly varies dramatically for different elements and has to be balanced. Isogeometric finite element analysis uses higher-order and smooth spline basis functions that exhibit higher-order continuity between elements, with support over a large number of Bézier elements. This leads to a consistently high bandwidth and large population of the system matrix. When classical element-wise parallelization approaches are used, these properties leads to prohibitively large communication between processes, which seriously affects parallel performance. In this work, we present an approach for massively parallel higher-order immersed domain and isogeometric finite element analysis. The key components of our methods are as follows: (1) we use a decomposition of the element matrix calculations to completely avoid communication during assembly, independent of the polynomial order and continuity of the basis functions; (2) we use a graph decomposition based on a distribution strategy to provide equal load per cluster node; (3) we rely on cache and memory-aware computation offload to integrate the processing power to coprocessors efficiently. We show several examples of immersed domain and isogeometric computations run on machines of the Minnesota Supercomputing Institute that demonstrate an increased parallel performance of our approach as compared to standard element-wise parallelization.

Title: Efficient Algorithms for Forward and Inverse Modeling of Multilayered Waveguides and Half-Spaces

Author(s): Ali Vaziri Astaneh, Murthy Guddati, *North Carolina State U.*

Guided wave propagation has been widely used in the contexts of geophysical inversion and nondestructive evaluation (NDE) through dispersion analysis. Motivated by the need for efficient computation of dispersion curves for layered media, a novel discretization approach, termed complex-length finite element method (CFEM), is developed and shown to be more efficient than the existing finite element approaches [1]. The new approach is exponentially convergent based on two key features: unconventional bending of the mesh into complex space and midpoint integration for evaluating the contribution matrices. For modeling layered half-spaces of infinite depth, we couple CFEM with perfectly matched discrete layers (PMDL) to minimize the errors due to mesh truncation. It is shown that the suggested combination of CFEM and PMDL drastically reduces the overall computational cost due to exponential convergence and sparse computation associated with linear finite elements, while requiring minor modifications to the existing finite element codes. Besides accelerating forward computation, we present a procedure to analytically differentiate the observed dispersion curve, which is obtained from frequency-wavenumber transformation of surface response measured at sparse locations, typical for geophysical inversion and NDE [2]. It is shown that the proposed differentiation approach is more efficient and accurate than the existing (finite difference) techniques, thus resulting in effective computation of Jacobian in the contexts of gradient inversion. A number of numerical experiments are utilized to verify the efficiency of the proposed methods and it is concluded that they lead to significant improvements in both gradient based and heuristic inversion of waveguides and half-spaces. [1] A. Vaziri Astaneh, M.N. Guddati, Efficient Dispersion Curve Calculation for Multilayered Waveguides and Half-Spaces, Submitted to Computer Methods in Applied Mechanics and Engineering. [2] A. Vaziri Astaneh, M.N. Guddati, Improved Algorithms for Inversion of Surface Waves Using Multistation Analysis, To be submitted to Geophysical Journal International.

Title: A Solution-Preserving Remeshing and State Mapping Procedure for Large Deformations

Author(s): Michael Veilleux, James Foulk, John Emery, Alejandro Mota, Jakob Ostien, *Sandia Nat'l. Lab.*

The focus of this presentation is on a robust methodology for remeshing and state variable mapping that preserves the solution with increased remeshing/mapping iterations for bodies subjected to large, nearly isochoric deformations. The remeshing scheme operates on either a global or local region wherein a high quality target mesh is generated in the current configuration that is topologically independent from the source mesh. This approach necessitates state variable transfers that: (1) operate on either globally or locally remeshed regions; (2) assume independent mesh topologies between source and target meshes in the remeshed regions; (3) preserve the solution; and, (4) update the kinematics for establishing a new reference configuration. Internal variables are transformed into their Lie algebras for addition[1], then extended through a global L2 projection and interpolated while maintaining their original spaces. The methodology is independent of element type, but a composite tetrahedral element is chosen for robustness in remeshing and accurate representation of nearly isochoric deformations[2]. Lightweight, parallel software applications have been implemented to necessitate efficient prototyping. The methodology is demonstrated and evaluated for a problem that requires remeshing and mapping: the complex deformation of a square bar far into the necking regime. References: [1] A. Mota, W. Sun, J.T. Ostien, J.W. Foulk III, K.N. Long. Lie-group interpolation and variational recovery for internal variables. *Computational Mechanics*, 52(6):1281-1299, 2013. [2] J.T. Ostien, J.W. Foulk III, A. Mota. A 10-node composite tetrahedral finite element for solid mechanics. In preparation. *Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Title: Bayesian Calibration & Validation of Soft Tissue Constitutive Models

Author(s): Kumar Vemaganti, Sandeep Madireddy, *U. Cincinnati*; Bhargava Sista, *ANSYS, Inc.*.

Constitutive models of soft tissue mechanical response are widely used in biomedical and biomechanical applications. These constitutive models are generally based on data from experiments such as compression, tension, indentation, etc. The high variability in these data leads to large variability in the constitutive model parameters, particularly when the problem of interest involves irreversible and discontinuous phenomena like tissue fracture and damage, as in injury biomechanics. When the uncertainties in the model parameters are ignored, it calls into question the reliability of the simulation that uses this constitutive model. In this talk, we discuss the use of a Bayesian approach to calibrating and validating soft tissue constitutive models. This approach combines prior knowledge of a model and its parameters with new experimental data to update the model and its predictions. We focus our attention on quantifying uncertainties in macroscopic constitutive models of soft tissue and propagate these uncertainties to simulations of soft tissue response. In particular we emphasize continuum constitutive models based on hyperelasticity, viscoelasticity and damage mechanics. We also demonstrate the use of Bayesian inference in optimizing soft tissue mechanical testing. The modeling is supported by experimental data from brain and liver tissue mechanical testing.

Title: On the Prediction of Turbulent Diapycnal Mixing in Stably Stratified Geophysical Flows

Author(s): Subhas Karan Venayagamoorthy, *Colorado State U.*

Two key quantities that are essential for estimating turbulent mixing in stably stratified flows are: the dissipation rate of the turbulent kinetic energy and the mixing efficiency, which is a measure of the amount of turbulent kinetic energy that is irreversibly converted into background potential energy. A linear relationship between the Thorpe (vertical overturn) length scale and the Ozmidov scale is widely assumed in oceanography to infer the dissipation rate of turbulent kinetic energy. This approach is particularly attractive since the vertical scales of overturns are easily calculable using a sorting algorithm from inversions in standard density profiles obtained from Conductivity-Temperature-Depth (CTD) measurements in the ocean. Hence the Thorpe scale is essentially a kinematic scale that provides a description of the turbulence at a given sampling location and instant in time. On the other hand, The Ozmidov scale is obtained from dimensional reasoning based on the assumption that there is a balance between inertial and buoyancy forces. In other words, the Ozmidov scale is a representative dynamic length scale of the largest eddy that is unaffected by buoyancy. A review of a number of recent studies will be presented in this talk to highlight the lack of a linear relationship between the Thorpe length scale and the Ozmidov scale. These studies indicate that inferred estimates of the dissipation rate of turbulent kinetic energy may be biased high by up to an order of magnitude or more especially for large overturns in the ocean. An alternative framework using a two-dimensional parameter space based on a buoyancy strength parameter (i.e. an inverse Froude number) and a shear strength parameter will be presented to characterize the scaling correspondence of the overturning scale with pertinent turbulent length scales. A discussion on the mixing efficiency and implications for estimates of diapycnal mixing in the ocean will be presented.

Title: Solution Reduction Approaches for the Variational Estimation of Cardiac Conductivities

Author(s): Alessandro Veneziani, Huanhuan Yang, Alessandro Barone, *Emory U.*; Flavio Fenton, *GA Tech.*

One possible strategy for estimating the cardiac conductivities is based on a variational data assimilation procedure. This consists of the constrained minimization (inverse problem) of a functional measuring the mismatch between available measures and numerical computations. The constraint is represented by the equations of electrocardiology (forward problem) that establish a link between conductivities and potential propagation. These equations are given by the Bidomain system for transmembrane and extracellular potentials. Preliminary results pointed out that the method may provide good estimates of conductivities even in real geometries. In addition, the same framework may be applied to multivariable assimilation, including the fiber orientation. However several theoretical and numerical issues were raised. The uniqueness of the solution to the constrained minimization problem is for instance an open problem. Another issue refers to the selection of the ionic model. We will show results of sensitivity analysis of the assimilation procedure to the selection of the ionic model. More specifically, some specific technical issues are met when using the so-called minimal model. The latter features discontinuous functions that require a special numerical treatment. However, the most important concern refers to the fact that this approach has a solid mathematical foundations yet has huge computational costs in particular in presence of regions with different conductivities like scars. This motivates the investigation of specific methods for reducing the computational costs. We address pitfalls and success of different possible approaches. In particular we explore solution reduction techniques based on a surrogate representation of the numerical solution built up on the online-offline paradigm. This approach was successfully used for estimating vascular compliance from medical images, as we will illustrate in the talk. However in electrocardiology they are problematic, since classical POD strategies are not effective for the slow decay of the singular values of the potential snapshots. We consider different ad-hoc reduced basis techniques that may provide a viable strategy in terms of computational efficiency. In addition, we present preliminary steps for an experimental validation of the entire procedure. Acknowledgement: NSF Project DMS - 1412973/DMS - 1413037, ``Collaborative Research: Novel data assimilation techniques in mathematical cardiology - development, analysis and validation". PI: A. Veneziani, F. Fenton.

Title: Mode-Based Inverse Identification of Turbine-Blade Geometry Using Surrogate-Based Optimization

Author(s): Vaibhav Yadav, Satchi Venkataraman, *San Diego State U.*; Scott Bland, *NextGen Aeronautics*.

Aircraft engines undergo survey testing to establish operation limits. Flow disturbances in the engine excite the blades. Engine survey testing provides information of blade vibration amplitudes over a range of engine speeds for the different excited modes. These amplitudes then are used to estimate stresses and determine fatigue life of components. The blade vibratory response in pristine conditions also provide baseline data for condition monitoring of the engine component and predicting the remaining life of safe operation [1]. However, the vibratory responses recorded by the end users can provide fatigue life estimates, only when they can be coupled with detailed finite element analyses if the components [2]. Often the end user of the engine does not have access to detail geometry and material data to set up such analyses, which is considered proprietary information belonging to original equipment manufacturer. This paper investigates the use of inverse identification of design of a rotor blade design details using some parametric geometry descriptors and measured blade vibratory response data. A surrogate-based optimization technique for performing mode-based inverse identification of blade geometry is presented. Challenges in developing an accurate surrogate model of the blade vibratory response, namely the calculated vibrations frequencies of the rotating blade in different modes and at varying rotational velocities (Campbell diagrams) are discussed. Different metrics using the optimization for matching of the calculated Campbell diagram with experimentally by measured Campbell diagrams are compared. The multi-dimensional surrogate model allows for efficient optimization leading to inverse identification and modal matching with the experimental data. References [1] Vsevolod Kharyton, Ronnie Bladh. Using Tiptiming and Strain Gauge Data for the Estimation of Consumed Life in a Compressed Blisk Subjected to Stall-Induced Loading. Proceedings of ASME Turbo Expo 2014: Turbine Conference and Exposition. June 2014, Dusseldorf, Germany. [2] Nichol, K. L. Assessment of current turbine engine high cycle fatigue test methods. Journal of engineering for gas turbines and power 125.3 (2003): 760-765.

Title: Mechanics-Based Characterization of Separation Force in Constrained-Surface-Based Photo-Polymerization Process

Author(s): Sonjoy Das, Abhishek Venketeswaran, Hang Ye, Chi Zhou, *U. Buffalo.*

Relative to the free surface (top-down) photo-polymerization or stereo-lithography (STL) based additive manufacturing (AM) process, the constrained-surface (bottom-up) STL based AM process has several advantages that include better vertical resolution, higher material filling rate, less production time, and less waste of photopolymer materials. Despite the advantages, one of the major concerns of the STL based AM process is that the fabricated part may break due to the resultant force generated during the pulling-up or separation process. This resultant force may become significant if the adhesive mechanism between the two contact surfaces (i.e., the newly cured layer and the bottom of the resin vat) induces a strong bonding characteristic. The main objective of the current work is to study the separation process from a mechanics perspective. This is done by modeling the adhesive mechanism between two different materials based on the concept of cohesive zone model (CZM), that has been successfully employed to study the crack propagation behavior in the field of fracture mechanics, and then simulating the separation process through finite element (FE) method. The separation process is equivalent to the damage evolution process in crack propagation study. Several user-defined and experimentally characterized cohesive laws currently exist in the literature. The cohesive laws define the traction between the two contact surfaces as mathematical functions of the separation/opening between the two interacting contact surfaces. The existing cohesive laws are, however, found to be unsuitable to characterize the experimental data obtained for different pulling-up speeds. In particular, the traction between the two contact surfaces is over-predicted, thus, compromising throughput of the STL based AM process. To mitigate this problem, a new cohesive law with strain-rate or velocity-dependent parameters is proposed in the present work. These parameters are estimated from the experimental data. The experimental data, however, show variability that, in turn, induces variability in the proposed cohesive law by making the velocity-dependent cohesive parameters as random variables. These random variables are next characterized within a polynomial chaos (PC) framework. The corresponding PC representations are constructed from the available experimental data. Cross-validation of the proposed method has also been carried out by comparing the probabilistic model predictions with the experimental data under different pulling-up speeds to validate the proposed method.

Title: Model-Order Reduction and Error Estimation for Variational Inequalities and Optimal Control

Author(s): Karen Veroy, Eduard Bader, Martin Grepl, Mark Kaercher, Zhenying Zhang, *RWTH Aachen*.

The reduced basis method is a model order reduction technique for the rapid and reliable solution of parametrized partial differential equations, and it is especially suited for the many-query, real-time, and slim computing contexts. This talk begins with a brief introduction into the basic elements of the RB method: approximation, a posteriori error estimation, offline-online computational decomposition, and a greedy algorithm. We then tackle some recent developments on a posteriori error estimation for the reduced basis method. We focus especially on two problem classes: variational inequalities and optimal control. In the first part, we discuss recent work motivated by variational inequalities in contact mechanics. We present here a duality approach that allows computation of error bounds that are significantly sharper than existing approaches. Furthermore, the proposed bounds are online-efficient --- that is, the computational cost depends only on the (low) dimension of the reduced problem. This is in contrast to existing approaches in which the cost depends on the (high) dimension of the original finite element problem. In the second part, we discuss recent work on model order reduction for optimal control problems governed by parametrized elliptic PDEs. Here, the reduced basis method is used as a low-dimensional surrogate model to solve the optimal control problem. We present a recently proposed error estimation procedure that provides bounds for the error in the optimal control and the associated cost functional. Numerical tests show that this proposed bound is not only efficient, but is also sharper and less sensitive to the regularization parameter than existing approaches. Finally, we combine the above-mentioned approaches to optimal control problems with control constraints.

Title: Positivity-Preservation Property of Cell-Centered Lagrangian Schemes and Extension to High-Orders of Accuracy

Author(s): Francois Vilar, Chi-Wang Shu, *Brown U.*

One of the main issue in the field of numerical schemes is to ally robustness with accuracy. And considering gas dynamics, at high Mach numbers or for flows near vacuum numerical approximations may generate negative density or pressure, which may lead to nonlinear instability and crash of the code. This phenomenon is even more critical using a Lagrangian formalism, the cells moving and being deformed during the calculation. In this talk, we first demonstrate in the two-dimensional case the positivity preservation property of a whole class of first-order finite volume cell-centered Lagrangian schemes, on generic curvilinear polygonal meshes, for different equations of states. This analysis enables us to derive time step conditions ensuring the desired positivity property as well as a L_1 stability of the specific volume and total energy over the domain. Adapting the work presented in [zhang,cheng] to the cell-centered Lagrangian frame, this positivity study is then extended to high-orders of accuracy. New time step constraints are then obtained, and a proper limitation is also needed. Through this new procedure, the scheme robustness is highly improved and hence new problems can be tackled. Numerical results are provided to demonstrate the effectiveness of these methods. [cheng] J. Cheng and C.-W. Shu, "Positivity-preserving Lagrangian scheme for multi-material compressible flow". J. Comp. Phys., 257:143-168, 2014. [despres] G. Carré, S. Delpino, B. Després and E. Labourasse, "A cell-centered Lagrangian hydrodynamics scheme in arbitrary dimension". J. Comp. Phys., 228:5160-5183, 2009. [maire] P.-H. Maire, R. Abgrall, J. Breil and J. Ovadia, "A cell-centered Lagrangian scheme for two-dimensional compressible flow problems". SIAM J. Sci. Comp., 29:1781-1824, 2007. [zhang] X. Zhang, Y. Xia and C.-W. Shu, "Maximum-principle-satisfying and positivity-preserving high order discontinuous Galerkin schemes for conservation laws on triangular meshes". J. Sci. Comp., 50:29-62, 2012.

Title: Level-Set XFEM Topology Optimization of 3D Navier-Stokes and Scalar Transport Problems

Author(s): Hernan Villanueva, *U. Colorado-Boulder.*

This presentation studies a topology optimization for incompressible Stokes and Navier-Stokes flow and scalar transport problems. The geometry of the flow domain is described by a level-set method (LSM) and the flow is predicted by the eXtended finite element method (XFEM). The study expands on previous work on the LSM-XFEM optimization framework by [1] to three-dimensions. The focus of this study is on the analysis of the boundary conditions along the fluid-solid boundary when considering moderate to high Reynolds number flow in the optimization problem. The velocity and pressure fields in intersected elements are approximated by an Heaviside enrichment strategy. Nitsche's method [2] is adopted to weakly impose Dirichlet boundary conditions on the velocity field. Ghost penalty terms capturing jumps in the spatial gradients of the velocity and pressure fields are added to improve stability and the conditioning of the system. This approach was previously applied to incompressible Navier-Stokes flows using face-oriented fluid stabilizations for both viscous and convective dominated flows. In this study, the method is expanded onto a generalized enrichment strategy and applied to convective transport problems. We demonstrate the robustness of the XFEM formulation for complex geometric configurations, as they often emerge in topology optimization. Design optimization studies illustrate the importance of imposing boundary conditions in both an accurate and robust fashion when optimizing the layout of flow channels at moderate to high Reynolds numbers. [1] Makhija D, Maute K (2014) Level set topology optimization of scalar transport problems. *Structural and Multidisciplinary Optimization* DOI 10.1007/s00158-014-1142-7 [2] Burman E, Hansbo P (2012) Fictitious domain finite element methods using cut elements: II. a stabilized Nitsche method. *Applied Numerical Mathematics* 62(4):328–341 [3] Schott B, Rasthofer U, Gravemeier V, Wall W (2014) A face-oriented stabilized Nitsche-type extended variational multiscale method for incompressible two-phase flow. *International Journal for Numerical Methods in Engineering*

Title: PyFR: High-Order Accurate Computational Fluid Dynamics on Unstructured Grids

Author(s): Peter Vincent, *Imperial College London*.

In this talk I will present PyFR (www.pyfr.org) [1], an open-source Python based framework for solving advection-diffusion type problems using the Flux Reconstruction (FR) [2] approach. The framework is designed to solve a range of governing systems on mixed unstructured grids containing various element types. It is also designed to target a range of hardware platforms via use of a custom Mako-derived domain specific language. Specifically, the latest release of PyFR is able to solve the compressible Euler and Navier-Stokes equations on grids of quadrilateral and triangular elements in two dimensions, and hexahedral, tetrahedral, prismatic, and pyramidal elements in three dimensions, targeting clusters of multi-core CPUs, NVIDIA GPUs (K20, K40 etc.), AMD GPUs (S10000, W9100 etc.), and heterogeneous mixtures thereof. Performance and accuracy studies will be presented for various benchmark and 'real-world' unsteady flow problems running on a range of systems, including heterogeneous mixed-platform workstations, and clusters with 100s of NVIDIA GPUs. Also, the performance and accuracy of PyFR will be compared with that of an industry-standard second-order flow solver across a range of problems. Throughout the talk the importance of algorithm-software-hardware co-design, in the context of next-generation computational fluid dynamics, will be highlighted. [1] Witherden, F. D., Farrington A. M., Vincent P. E., PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach, *Computer Physics Communications*, 185(11) pp. 3028-3040, 2014. [2] Huynh, H. T., A Flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods, *AIAA Paper* 2007-4079, 2007.

Title: Evaluation of Vortex-Blade Interaction Utilizing Flow Feature Detection Techniques

Author(s): Nuno Vinha, Eusebio Valero, *U. Politécnica de Madrid*; David Vallespín, Valentin de Pablo, *Airbus Operations S.L.*

The extraordinary growth of computational capabilities over the last few decades has enabled the numerical simulation of massive and complex flow problems with high accuracy. Not surprisingly, CFD has become a crucial tool in the design of pioneering aircraft engine architectures. An example of such innovation is the Counter-Rotating Open Rotor (CROR) project, aiming to enhance fuel consumption and emissions over conventional turbofan engines. Noise and performance requirements lead the design process from a very early stage, thus requiring deep investigation of the acoustic and aerodynamic behavior. Monitoring the trajectory of the vortices generated at the tip of the front rotating blades is of critical importance to understand and prevent tip-vortex impact with subsequent rotor stages. This non-linear flow topology strongly influences the aerodynamic performance and acoustic footprints, and needs to be evaluated over a wide range of flight conditions. More specifically, there is a necessity to predict possible sources of tonal and broadband noise due to tight noise regulations within the airspaces. They can be directly associated to vortex-blade interactions and broken-down vortices, respectively. An effective and efficient tracking of these coherent structures is therefore indispensable to the designers that look for advantageous configurations. Full annulus, uRANS simulations of an industrial CROR test-case produce large amounts of raw data that needs to be post-processed. Searching for meaningful rotational structures through the entire dataset, by means of classical direct visualization techniques, might result in a fruitless and inefficient effort. Alternatively, the identification of relevant vortices emerging in this three-dimensional, large scale unsteady problem becomes much more straightforward when following a flow feature detection oriented approach. By increasing the data's level of abstraction, the researcher is able to achieve an important data size reduction. This allows for faster and more accurate analysis with lower uncertainties without requiring excessive additional computational costs. One of the objectives of this paper is to evaluate the suitability of traditional region and local-based vortex detection techniques, available in the open literature, for the particular case of CROR. The evaluation of the strengths and weaknesses of each individual algorithm and its computational performance revealed decisive insights into a new coupling methodology which is also presented in this paper. This new method provides automatic feedback about the vortex-blade impact or no-impact condition. This should result in a more efficient procedure for the design-to-noise iterative process.

Title: Treating a Vesicle Membrane as an Immersed Boundary to Simulate Cell Desiccation

Author(s): Chris Vogl, *U. Washington*.

Lyopreservation seeks to store biological tissues by desiccation instead of traditional freezing techniques. During the drying process, however, the cell membrane can undergo large deformations that lead to cell death. Thus, the mechanics of a vesicle membrane are simulated in order to understand optimal drying conditions. The membrane is modeled as a bending resistant, inextensible interface within a fluid containing a desiccant. The numerical approach includes level set, immersed boundary, immersed interface, and closest point type methods.

Title: Modeling Dynamic Stimulation of Geologic Resources

Author(s): Oleg Vorobiev, Joe Morris, Eric Herbold, Bradley White, *LLNL*.

Dynamic loading methods promise new modes for stimulating geological resources. In contrast to traditional fracturing methods (e.g. hydraulic fracturing) the stresses in the source region may be significantly larger than the insitu stress which helps creating fractures not oriented with the maximum insitu stress. This paper discuss simulation of dynamic fracture initiation and propagation using Lawrence Livermore's GEODYN-E and GEODYN-L codes. These are massively-parallel multi-material codes developed for shock wave propagation in heavily jointed rock masses. The codes have been validated by modeling various underground explosions over the years. We focus on various mechanisms of dynamic fracture generation in a rock formation with pre-existing joints/cracks. Various source geometries and energy release rates are considered to optimize the enhancement of the fracture network, which could be stimulated later using traditional methods.

Title: Crack Propagation Analysis with Fracture Surface Contact Under Torsional Loading

Author(s): Yoshitaka Wada, *Kindai U.*

Crack growth under the elastic-plastic fracture is an important issue of the structural integrity, because seismic wave causes low cycle fatigue in the engineering structure. Many researchers have worked for many experiments and numerical analyses, however obvious and general criterion cannot be found until now. In order to develop a three-dimensional fracture criterion, the fully automated and state-of-the-art FE crack growth simulation should be realized. In the numerical simulation system, there are three important processes which are generation of the model with crack, stable and accurate FE analysis and post-processing for fracture evaluation. Crack growth simulation requires each process to be stable and connected each other in the one system. On the other hand, experiment should be conducted to determine material properties such as cyclic stress strain curve, crack tip opening displacement, J integral and so on. In particular, determination of parameters for appropriate cyclic stress strain curve is very important to actual evaluation of seismic loading. We developed automated FEM analysis framework for elastic-plastic crack growth simulation. The framework consists of 4 major modules. The first module is the determination of the parameters for constitutive equation. The second module is the mesh generation with cracks. Crack tips move to the direction which is determined by three-dimensional fracture criterion. According to crack tip movement, the mesh also is regenerated by the automatic mesh generator. The third module is nonlinear finite element application. In this study we employ ANSYS 11. We define the data structures between each module and specifications of the framework. Therefore, the framework can accept the other FE codes for elastic-plastic crack growth simulation. The last module is the evaluation of fracture parameters to evaluate crack growth direction and rate. In this work, we employ crack tip opening displacement (CTOD) and crack tip opening angle (CTOA) which are the geometrical parameters to be defined near the crack tip. The present work shows the result of contact analysis of a pipe with a single notch at the low cycles, because contact behavior of crack surfaces occurs under the applied cyclic loading in the past work. In order to show the effectiveness of CTOD and CTOA parameters in the pipe, the conventional generation phase and application phase analyses are conducted. The work shows comparisons between experimental result and numerical simulation results. We discuss the effectiveness of fracture mechanics parameters for crack growth criterion under torsional cyclic loading.

Title: A Multi-Temporal Scale Approach to the Fatigue Life Prediction of Rubber

Author(s): Shogo Wada, Dong Qian, *UT Dallas*.

Fatigue failure of rubbery materials dominates the life of many manufacturing products, e.g., engine mount, tire, seismic isolation rubber, etc. However, prediction of fatigue damage or crack propagation in rubber remains a challenging problem due to the large time scale involved in the application as well as the lack of accurate modeling tools. In this presentation, we present a multi-temporal scale approach to the life prediction in rubbers. The approach is motivated by the idea of establishing approximations in both the spatial and temporal domains in the context of space-time finite element formulation. By integrating the time discontinuous Galerkin approach with the enrichment scheme (Bhamare, Eason et al. 2013), we show that the method is robust in resolving material responses under dynamic loading conditions that are commonly encountered in the application of rubber. To capture fatigue failure, the proposed multi-temporal scheme is further integrated with a damage modeling scheme that is developed for rubbery materials. After outlining the basic computational framework, example problems are provided to demonstrate the application of the method. Acknowledgement: S. Wada would like to thank the Bridgestone Co. for a fellowship of the graduate study. References Bhamare, S., T. Eason, S. Spottswood, S. Mannava, V. Vasudevan and D. Qian (2013). "A multi-temporal scale approach to high cycle fatigue simulation." *Computational Mechanics*: 1-14.

Title: Enhancing Groundwater Quality Through Computational Modeling and Simulation to Optimize Transport and Interaction Parameters in Porous Media

Author(s): Akhil Waghmare, *Thomas Jefferson H.S. Sci. & Tech.*; Padmanabhan Seshaiyer, *George Mason U.*

There is a shortage of high quality drinking water caused by the introduction of contaminants into aquifers from various sources including industrial processes and uncontrolled sewage. Studies have shown that colloids, collections of nanoparticles, have the potential to remediate polluted groundwater. For such applications of nanoparticles, it is important to understand the movement of colloids. This study aims to enhance the previously developed MNM1D (Micro- and Nanoparticle transport Model in porous media in one-dimensional geometry) by making more realistic assumptions about physical properties of the groundwater-porous medium system by accounting for a non-constant flow velocity and the presence of electromagnetic interactions. This was accomplished by coupling the original model with the Darcy-Forchheimer fluid model, which is specific to transport in porous media, coupled with electromagnetic effects. The resulting model also accounts for attachment and detachment phenomena, both of the linear and Langmuirian type, as well as changes to hydrochemical parameters such as maximum colloidal particle concentration in the porous medium. The system of partial-differential equations that make up the model was solved using an implicit finite-difference discretization along with the iterative Newton's method. A parameter estimation study was also conducted to quantify parameters of interest. This more realistic model of colloid transport in porous media will contribute to the production of a more efficient method to counteract contaminants in groundwater and ultimately increase availability of clean drinking water.

Title: Optimal Conjugate Heat Transfer Coupling Through a Dirichlet-Robin Boundary Condition

Author(s): Gregory Wagner, *Northwestern U.*; Victor Brunini, *Sandia Nat'l. Lab.*.

Predicting the reaction and decomposition of foam or other organic materials is an important problem in ensuring the safety of certain systems under extreme thermal conditions such as fire. This is a complex multi-physics problem that includes flow through a reacting porous material with a moving interface coupled to surrounding fluid and solid domains through mass, energy, and species transfer at the boundaries between materials. We demonstrate that this problem can be solved through a fully coupled monolithic matrix solution, but it has been found that more efficient segregated approaches can lead to loss of stability. Furthermore, the two-temperature (solid and fluid) model of the porous regions leads to ambiguities in traditional treatments of the coupled boundary conditions. Motivated by this problem, we explore new forms of the conjugate heat transfer coupling boundary condition that can be used at these interfaces. We derive an optimal coupling parameter for a Dirichlet-Robin form of the time-dependent conjugate heat transfer coupled boundary condition, and show that a modification of the capacitance matrix is necessary in order to converge to the same solution as the fully coupled case.

Title: A Coupled Phase-Field, Shear Band Model for Dynamic Fracture

Author(s): Colin McAuliffe, Haim Waisman, *Columbia U.*

Dynamic fracture of metals may be brittle or ductile depending on factors such as material properties, loading rate and specimen geometry. At high strain rates, a thermo plastic instability known as shear banding may occur, which typically precedes fracture. Experiments on notched plate impact show a ductile - brittle failure transition, where lower impact velocities lead to brittle behavior, while higher impact velocities lead to shear banding. For more complex problems such as armor penetration, both brittle fracture and shear banding have been observed in the same specimen, however, current failure models can either account for fracture or shear banding. For predictive numerical simulations of dynamic failure, it is thus crucial to account for both failure modes, since exclusion of either mode neglects important physics observed in experiments. In this work a thermodynamically consistent model which accounts for both shear banding and dynamic fracture and can thus capture both failure modes at intermediate strain rates, is presented. The model consists of an elastic-viscoplastic material with strain hardening, strain rate hardening, and thermal softening. Fracture is modeled with the phase field method, for which a novel modification is presented here to account for the creation of fracture surfaces by inelastic work. We will present the main formulations along with some numerical examples to illustrate the basic behavior of the model. [1] Colin McAuliffe and Haim Waisman, A unified model for metal failure capturing shear banding and fracture, *International Journal of Plasticity*, 65:131-151, 2014. [2] Luc Berger-Vergiat, Colin McAuliffe and Haim Waisman, Isogeometric Analysis of Shearbands, *Computational Mechanics*, 54(2):503-521, 2014. [3] Colin McAuliffe, and Haim Waisman, Mesh insensitive formulation for initiation and growth of shear bands using mixed finite elements, *Computational Mechanics*, 51(5):807-823, 2013.

Title: Uncertainty Quantification and Statistics Based Material Modeling for Complex Biomechanical Problems Exemplified for AAA

Author(s): Wolfgang A. Wall, Jonas Biehler, Michael Gee, *TUM*.

The use of computational models in a clinical setting for diagnostic and predictive purposes of course requires truly patient-specific models. However, many parameters in such models exhibit significant inter- as well as intra-patient variations. In spite of these sometimes drastic variations, most researchers have hitherto condensed the extensive experimental findings to population averaged mean values, which are then used as input parameters for computational models. While the use of deterministic models with averaged parameters has its merits, the predictive capability of these models is often limited. We believe that the predictive capabilities of computational simulations can be enhanced if the aforementioned variations are considered in the computational assessment. This can be achieved by using a probabilistic description for the varying parameters and an efficient uncertainty quantification (UQ) framework. Thereby, the available experimental data should be used to construct the probabilistic description of the uncertain parameters. In this work, we present a framework for efficient UQ in large scale, nonlinear biomechanical problems with high stochastic dimension. This allows us, for the first time, to perform UQ using patient-specific models with respect to multiple uncertain parameters, which are modeled as random fields. Moreover, we demonstrate the utility of a data driven approach for the construction of patient-specific random fields for uncertain model parameters. Furthermore, by comparison to the results obtained with a simpler random variable model, the necessity to consider intra-patient variations of the parameters is evaluated. Although the developed approach is very general and can easily be applied to a large variety of biomechanical problems we will use Abdominal Aortic Aneurysms (AAA) as a specific demonstrator example in this talk. Specifically, we investigate the impact of uncertainties in constitutive parameters and wall thickness on mechanical quantities typically related to AAA rupture risk, such as wall stress or strain. The probabilistic description for the uncertain parameters is thereby, to a large extend, determined from extensive experimental data. In this context will briefly show how advanced regression techniques can be used to predict such parameters and notably reduce input uncertainties. Biehler, J., Gee, M.W., Wall, W.A., Towards Efficient Uncertainty Quantification in Complex and Large Scale Biomechanical Problems Using Approximate Models and Bayesian Formulations, *Biomechanics and Modeling in Mechanobiology* 2014 doi:10.1007/s10237-014-0618-0 Biehler, J., Kehl, S., Gee, M.W., Tanios, F., Pelisek, J., Maier, A., Reeps, C., Eckstein, HH., Wall, W.A., Non-Invasive Prediction of Wall Properties of Abdominal Aortic Aneurysms Using Bayesian Regression, submitted 2015

Title: An Operator-Based Framework for Inverse Problems

Author(s): Timothy Walsh, *Sandia Nat'l. Lab.*

Inverse problems are frequently encountered in acoustic, structural, and structural acoustic applications. Given measured accelerometer or microphone time histories, one may need to estimate material properties in a structure, impedance conditions on the boundaries, shape or topology of an object, or characterize acoustic and structural sources that produced the measured data. Applications include model calibration, acoustic testing of aerospace structures, military surveillance, and medical diagnostics. Typically, accelerometer or microphone pressures are measured experimentally, and it is desired to characterize the material parameters, boundary conditions, topology, or acoustic sources that produced these accelerations or microphone pressures. Many of these applications of interest involve large acoustic domains and high frequency ranges, thus making a massively parallel implementation essential. In this talk we will present a parallel, operator-based partial differential equation (PDE) constrained optimization approach that results from the first-order optimality or Karush-Kuhn-Tucker (KKT) conditions. We will present the specific forms of these operators resulting from time-domain, frequency-domain (Helmholtz), and eigenvalue (modal) domain formulations, where one may be interested in inverting for material properties, loads, and/or Robin boundary conditions. The merits and drawbacks of the different domains will be discussed and compared. This abstract framework enables one to reduce any inverse problem to a set of fundamental operations and enables re-use of several software constructs. The operator-based strategy provides a natural interface to Sandia's Rapid Optimization Library (ROL), which will be presented and discussed. 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-AC04-94AL850000.

Title: A Coupled ALE-AMR Approach to Shock Hydrodynamics on Tetrahedral Grids

Author(s): Jacob Waltz, Jozsef Bakosi, *Los Alamos Nat'l. Lab.*

Arbitrary Lagrangian-Eulerian (ALE) and Adaptive Mesh Refinement (AMR) algorithms are well-established techniques for the simulation of shock hydrodynamic problems. ALE methods are often implemented in a Lagrange-plus-remap framework to maintain mesh robustness during extreme fluid distortion, whereas AMR methods are typically implemented in an Eulerian framework to increase mesh resolution at discontinuities. However, despite their individual records of success, very few examples of coupled ALE-AMR methods can be found in the literature, and none address unstructured grids. In this work we describe an approach to coupled ALE-AMR simulation of shock hydrodynamics problems, as applied to three-dimensional meshes consisting of unstructured tetrahedral cells. In the coupled methodology the unstructured grid is able to move with the flow as in a traditional ALE method, but also simultaneously refine at – and derefine away from – discontinuities. The combined approach is implemented within the context of a node-centered discretization using linear Finite Element basis functions and an unsplit time integration of the ALE hydrodynamic equations. The unique challenges required to achieve a robust and mathematically consistent coupling of the two algorithms are discussed. These challenges include: mesh relaxation across AMR boundaries; robust motion of fine-level mesh cells; conservation of volume during derefinement; and appropriate error estimates. The specific techniques used to overcome each of these challenges are described. The resultant algorithm brings the benefits of AMR, that have heretofore been leveraged almost exclusively by Eulerian simulations, to moving grid solution approaches. We also discuss how the individual weaknesses of ALE and AMR can be overcome by a coupled methodology. For example, ALE methods can create coarse mesh regions as a consequence of concentrating mesh points near flow features. Secondary flow phenomena (e.g. reflected shocks) can then transport through these coarse mesh regions, with high numerical errors that could be mitigated through AMR. The coupled ALE-AMR approach has been applied to a number of standard shock hydrodynamics test problems. Comparisons to AMR-only and ALE-only simulations on the basis of both accuracy and time-to-solution for a given level of error will be included.

Title: Computational Study of Cortical Convolution Patterns in a Developing Brain

Author(s): Mir Jalil Razavi, Tuo Zhang, Tianming Liu, Xianqiao Wang, *U. Georgia.*

Soft tissues are complex materials with typical nonlinear, anisotropic, inhomogeneous behaviors subjected to large strains and stresses. Growth or atrophy of soft materials in media may lead to instability and formation of surface wrinkling, folding or creasing which depends on a variety of factors such as geometry and material properties. Instabilities in the soft materials to adjust the shape configuration and dictate morphological evolution is playing a crucial role in the healthy behavior of soft biological tissues. Convolutional cortical folding, characterized by convex gyri and concave sulci, has an intrinsic relationship to the brain's functional organization. Understanding the mechanism of convolution patterns can provide useful insight into normal and pathological brain functioning. However, despite decades of speculation and endeavors the underlying mechanism of the folding process remains poorly understood. Most famous hypotheses in this area are related to the roles of differential expansion of the cortex, radial growth, and internal tension in neuronal fibers. In the differential growth hypotheses, which we consider it in this paper, outer layers of the brain grow at faster rates than the inner layers, acting as the driving mechanism of cortical folding. Based on the differential growth hypothesis, a soft double-layer hyperelastic sphere model with outer cortex and inner core is modeled as the developing human brain so as to imitate the growth. In analytical part both deformation and stress fields inside the brain are derived and analyzed. Analytical interpretations for isotropic growth of the brain model provide preliminary insight into critical growth ratios for instability and sulcification of the developing brain with hyperelastic material, but it fails to predict the evolution of cortical complex convolution after the critical point. For overcome to this issue, in the computational part, non-linear finite element models based on finite growth are employed to present sulcification and secondary morphological folds of the growing brain. The results show that dependent on the cortex-to-core growth ratio, growth induces residual stresses in the material that often cause large enough compressive stress to initiate instability in the material. Initial thickness and material properties of the outer cortex relative to the inner core have a great effect on the morphological patterns of the growing brain. Based on results, special abnormalities in the fetal stage of a developing brain have been introduced, explained by models, and compared with experimental observations.

Title: The Long Time Dynamics Behavior of Richtmyer-Meshkov Instability and Turbulent Mixing

Author(s): Tao Wang, *Mianyang City*.

As a shock wave passes through a perturbed interface between two different flows, the baroclinic vorticity is deposited at the interface by the misalignment of pressure gradient of across the shock and the local density gradient at the interface, and causes the perturbed interface to grow. This phenomenon is named as the Richtmyer-Meshkov instability (RMI), which often happens in a variety of man-made applications and natural phenomena such as inertial confinement fusion (ICF), deflagration-to-detonation transition (DDT), high-speed combustion and astrophysics (i.e. supernova explosions). The RMI is so important that it has gained significant attention all long. When an incident shock wave impacts an initial corrugated interface in lighter/heavier configuration, it bifurcates into a reflected shock wave and a transmitted shock wave with decreasing intensity. The transmitted wave reverberates between the accelerated interface and the end-wall of shock tube and is refracted to form a process of multiple impingements. In this report, the dynamics behavior of the Richtmyer-Meshkov instability induced turbulent mixing under multiple impingements is investigated by using large-eddy simulation. Each impingement advances the development of turbulent mixing zone (TMZ) greatly and results in an abrupt change of turbulent mixing. However, the turbulent mixing zone grows in different manner for each impingement. After the initial shock, it grows as a power law of time. For the reshock and impingement of reflected rarefaction wave, it grows in time as a different exponential law. When the impingement of reflected compression wave completes, it grows approximately in a linear fashion. The statistics in turbulent mixing zone decay with time in the similar way to the width of TMZ under multiple impingements except for the impingement of reflected compression wave, after what the statistics decays asymptotically. It can be concluded that the turbulent mixing zone behaves in a way of statistics similarity. Even though the impingements of different waves result in a different abrupt change of the characteristic scale parameters of mixing turbulence, as a whole, the characteristic scales present a feature of growth, and the characteristic scale Reynolds numbers present a feature of decaying.

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Title: A New Implicit Direct Force Approach of Immersed Boundary Method for Simulating Complex Moving Boundary Flow

Author(s): Wen-Quan Wang, *Kunming U. Sci. & Tech.*; Fang-Bao Tian, *U. New South Wales*.

In the implicit direct forcing immersed boundary (IB) method [1], the force distribution and velocity interpolation are coupled in an implicit manner. The advantage of the implicit approach is that the velocity boundary conditions at the interface are satisfied more accurately than the explicit approaches. However, this method requires computational resources to solve the linear equations, which could be computationally expensive for problems involving large number of IB nodes or multiple immersed bodies. In this talk we will show how to implement a new implicit direct force approach of IB method for the problems involving moving boundaries and complex geometries. In this method, a higher-order discrete delta function [2] is used to spread the Lagrangian force exerted by IB points to surrounding Cartesian grids to suppress the non-physical oscillations. In addition, a fast solving method for boundary force density is incorporated. The resulting combination gives an easy-to-use, inexpensive and accurate technique which can be an important step towards the application of computational fluid dynamics to industrially relevant problems. To reduce the diffusion observed in the conventional full distribution (FD) forcing strategy, a half distribution forcing strategy ■HD is used to handle the velocity correction. The accuracy and capability of the present method are demonstrated by comparing the results by the different discrete delta functions with HD and FD forcing strategies method.

Title: High-Order Simulation of the Convection and Differential Rotation in Rapidly Rotating Stars

Author(s): junfeng wang, chunlei liang, *George Washington U.*

We have investigated the non-linear feedback between the convection, oblateness and differential rotation in rapidly rotating stars by extending our recently developed novel and powerful Compressible High-Order Unstructured Spectral-difference (CHORUS) code. Recent observations have revealed the drastic effects of rapid rotation on stellar structure. In rapidly rotating stars, the centrifugal force counteracts gravity, causing the equatorial region to expand. Consequently, rapidly rotating stars are oblate and the differential rotation will further deform the configuration. We extend our CHORUS code to model the rapidly rotating stars in 3D and to understand how they pulsate using deforming grid. In CHORUS code, the hydrodynamic equations are discretized by a robust and efficient high-order Spectral Difference Method (SDM) on unstructured grids. For the SD method, in the standard element, two sets of points are defined, namely the solution points and the flux points. The solution and flux values within the element can be computed using Lagrangian polynomials. On the cell interfaces, an approximate Riemann solver is used for computing inviscid flux and an averaging operation is used to compute viscous fluxes. The computational stencil of the spectral difference method is compact and advantageous for parallel processing. CHORUS demonstrates excellent parallel performance, scaling up to 12,000 cores on the Yellowstone High-Performance Computing cluster at National Center for Atmospheric Research (NCAR). The code is verified by defining two benchmark cases for global convection in Jupiter and the Sun. CHORUS results are compared with results from the Anelastic Spherical Harmonics (ASH) code and good agreement is found. In our 3D rapidly rotating star simulation, a total of 393,216 hexahedral elements are used.

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Title: A Three-Dimensional Field Formulation, and Isogeometric Solutions to Point and Line Defect Cores Using Toupin's Theory of Gradient Elasticity at Finite Strains

Author(s): Zhenlin Wang, Shiva Rudraraju, Krishnakumar Garikipati, *U. Michigan.*

We present a finite strain gradient elasticity based field formulation of point defects, edge and screw dislocations, and dislocation interactions. We have chosen for our work, Toupin's theory [Arch. Rat. Mech. Anal., 11(1), 385-414, 1962]— one of the more general formulations of strain gradient elasticity. Our framework has three crucial ingredients: The first is iso-geometric analysis [Hughes et al., Comp. Meth. App. Mech. Engrg., 194(39-41), 4135-4195, 2005], which we have adopted for its straightforward and robust representation of C1-continuity. The second is a weak treatment of the higher-order Dirichlet boundary conditions in the formulation, which control the development of strain gradients in the solution. The third ingredient is algorithmic (automatic) differentiation, which eliminates the need for linearization “by hand” of the rather complicated geometric and material nonlinearities in gradient elasticity at finite strains. We also present a number of numerical solutions to demonstrate that the framework is applicable to arbitrary boundary value problems in three dimensions.

Title: An All-Electron DFT Calculation Using Spectral Gauss Quadrature

Author(s): Xin Wang, *Army Rsch. Lab.*.

The conventional solution to the Kohn-Sham problem involves finding N lowest eigenvalues and eigenvectors, where N is the number of electrons in the system. Due to the orthogonality condition on the eigen-states, finding all N eigen-states is a computationally cumbersome task. The concept of pseudopotentials was introduced to reduce the computational cost by computing only the eigen-states that correspond to the valence electrons. In addition, the valence orbitals resulted from the pseudopotentials are smooth near the nuclei so that a coarser mesh or lower plane-wave cutoff could be used in computation as compared to all-electron calculations. Since the electrons do not separate strictly into core and valence electrons, depending on the type of atoms in the molecular system and the properties we want to compute, we have to choose a "softer" or "harder" pseudopotential. The alternative to using pseudopotentials is to perform all-electron calculations. All-electron calculations require at least an order of magnitude finer spatial discretization than pseudopotential calculations, as a result of the oscillatory behavior of the orbitals near the nuclei. We introduce a new way to reduce the computational cost of all-electron calculations using the linear scaling spectral Gauss quadrature (LSSGQ) method developed by Suryanarayana et al. [1]. The key idea behind the LSSGQ approximation is to represent quantities such as electron density and energy using spectral integrals of the Hamiltonian matrix, and approximate the integrals using spectral Gauss quadrature. The essential pieces of the LSSGQ method are the quadrature weights and nodes. Taking advantage of the scarcity of the Hamiltonian matrix, the computation of the spectral Gauss quadrature nodes and weights for each spectral integral can be evaluated at cost independent of the size of the system; resulting in a numerical scheme that scales linearly with respect to the system size. We take advantage of the fact that we can compute the spectral Gauss quadrature nodes and weights for each spectral integral subject only to a subset its neighboring nodes. We mimic the multi-mesh concept in the coarse-graining DFT method proposed by Suryanarayana et al. [1] and adapt the LSSGQ method to perform an all-electron calculation at computational cost that is significantly less than brute-force all-electron calculations. [1] Phanish Suryanarayana, Kaushik Bhattacharya, and Michael Ortiz. Coarse-graining Kohn-Sham Density Functional Theory. *Journal of the Mechanics and Physics of Solids*, 61(1):38–60, January 2013.

Title: A Few Thoughts on the Modeling of Complex Systems

Author(s): Sheldon Wang, *Midwestern State U..*

The key phenomenological law of complex systems often take the form of the power law. This is the manifestation of the fractal dimension in chaotic systems with many interactive factors. For instance, in the crack propagation, we have the Paris law, $da/dN=A (K_r)^B$, where the range stress intensity factor is related to the range nominal stress as $K_r=\sigma_r (\pi a)^{0.5}$, with a as the crack length; whereas in skin friction for laminar and turbulent boundary layers, we have the friction coefficient related to the Reynolds number as, $C_f=A (Re_x)^B$, where the Reynolds number Re_x is defined as Ux/ν , with U as the far field flow velocity, x as the length of the boundary layer, and ν as the kinematic viscosity of the fluid. Notice that from experimental validations, we can easily obtain A and B as 0.664 and 0.5 for laminar boundary layers and 0.0594 and 0.2 for turbulent boundary layers. Our computational simulation should produce bridges between these phenomenological laws for different scales for both concurrent and hierarchical models. The question might be what if we do not have phenomenological laws for these scales. We probably have to adjust our scales and redefine the governing variables. Examples will be presented to illustrate the concepts in this direction.

Title: Torsional Stability of Carbon Nanotubes Encapsulating Metal Atoms Using Atomistic Simulation

Author(s): Lei Wang, Hohai U..

In nanoelectromechanical systems (NEMS), torsional devices can be used for a wide number of applications including sensors, signal processors, optical modulators, clocks for electronics, and resonators, etc. Due to their excellent mechanical, electrical, and thermal properties, carbon nanotubes (CNTs) are expected to be the ideal candidate for use as torsional springs in NEMS. CNTs can also act as torsional electromechanical oscillators or rotational bearings in actuators. Furthermore, CNTs subjected to torsion can also serve as a channel for transportation of hydrogen molecules. Thus, it is important to gain a clear understanding about the torsional behavior of carbon nanotubes. The encapsulation of metal atoms into the internal cavity of carbon nanotubes may significantly alter their conducting, electronic and mechanical properties and create intriguing multifunctional nanodevices. Using classical molecular dynamics method, firstly, the induced torsion of single-walled carbon nanotubes filled with copper atoms is investigated under axial tension and compression. Results show that this coupling response between torsional deformation and axial strain is only limited to chiral filled tubes. As compared with the behavior of empty chiral tubes, due to the van der Waals interaction between tube wall and the encapsulated metal atoms, the induced torsional behavior of chiral filled tubes is reversed and its diameter dependency is contrary. Secondly, the buckling deformation of single-walled carbon nanotubes completely filled by copper atoms is studied under external torsion. Due to the metal filling, the torsional rigidity of tubes can be dramatically enhanced and the critical torsional angles of filled tubes can be 2~4 times higher than those of empty ones. Furthermore, due to structural asymmetry in chiral metal-filled tubes, there exists a dependency of the torsional behavior on loading directions. These results can provide helpful guidelines for the applications where carbon tubes serve as torsional devices.

Title: A Reliability Analysis Method for Crash and Impact Problems Using Augmented RBF Metamodels

Author(s): Qian Wang, *Manhattan College*; Hongbing Fang, Daniil Kuvila, *U. North Carolina-Charlotte*.

Reliability analysis of various crash and impact problems is a challenging task since expensive numerical simulations are generally required. To improve the computational efficiency of reliability analysis of these problems, a metamodeling technique based on augmented radial basis functions (RBFs) was investigated. The RBFs are suitable for creating accurate approximations (metamodels) for linear and nonlinear responses using a relatively small number of sample points (simulation runs). The RBF metamodels have a special advantage in terms of model accuracy, since the models have no errors at the sample points (i.e., pass through the sample points). In this study, augmented RBFs were used to create high-fidelity metamodels of a limit state/performance function. Once the RBF metamodels were generated, the failure probability was calculated using simulation methods such as Monte Carlo simulations (MCS). Mathematical and practical engineering examples were used as test examples to study different types of responses. Various sample sizes were tested and failure probabilities were calculated. The failure probability obtained based on the RBF metamodels was found to have good accuracy with a reasonable number of sample points. The proposed reliability analysis method based on augmented RBF metamodels was very efficient, especially for crash and impact problems involving expensive numerical simulations but the number of random variables is relatively small.

Title: Evaluation of Peridynamic Models for Damage and Failure in FRCs

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

Modeling of damage and failure in fiber-reinforced composites (FRCs) is a very challenging problem because of the complexity of the phenomenon. In FRCs, the micro-structure and anisotropy lead to complicated stress/strain states that are further influenced by interactions with elastic waves propagating in the structure. Some recent peridynamic (PD) models for FRCs ([1], [2]) have been able to simulate dynamic crack growth and failure of these materials. In this talk we discuss such models and compare their results for several tests cases. We first verify the models for wave propagation examples and then use them to model fracture and damage evolution. We perform the following tests cases: impact and intersonic crack propagation in unidirectional FRCs [3], and dynamic crack growth from quasi-static or dynamic loading of unidirectional FRCs. We find that PD models that try to mimic the macroscopic slowness curve (tension surface) at the PD microscale do not lead to failure modes seen in some experimental tests on FRCs. On the other hand, PD models that assume only two types of micro-bonds, similar to the actual two-phase composition of the FRC, are capable of reproducing, accurately, failure modes and crack propagation speeds seen in experiments. In particular, we discover an interesting phenomenon: a strong strain-rate dependence for the modes of failure in a unidirectional 45° FRC. In the slow-dynamic loading regime, we observe that the crack initiates and grows perpendicular to the loading direction, through the matrix, over the fibers, and without breaking them. Under high strain-rate loading, the crack initiates along the 45° fiber direction, leading to splitting-mode (fiber-matrix delamination) failure of the composite. We verify our model for a $\pm 45^\circ$ composite against experimental results, and the cracks propagate along $\pm 45^\circ$ in both simulation and experiment. References: [1] W. Hu, Y. D. Ha and F. Bobaru. *Journal for Multiscale Computational Engineering*. vol 9(6): 707-726, 2011. [2] M. Ghajari, L. Iannucci and P. Curtis. *Computer Methods in Applied Mechanics and Engineering*. vol 276: 431-452, 2014. [3] D. Coker and A. J. Rosakis. *Philosophical Magazine A*. Vol. 81 No. 3:571-595, 2001.

Title: From Diffuse Damage to Sharp Cracks: A Cohesive Extended Finite Element Framework for Crack Propagation

Author(s): Yongxiang Wang, Haim Waisman, *Columbia U.*

Abstract: The present work is devoted to the numerical simulation of crack propagation in quasi-brittle materials, whose failure can be idealized in two phases: diffuse material degrading process and strain localization up to the formation of strong discontinuity. Continuum damage mechanics provides an excellent framework to describe the first phase of material failure, but is unable to represent strong discontinuity arising in the damage localization phase. In sharp contrast, cohesive zone models can not describe the diffuse material damage process very well. However, discrete cracks are well represented in these models. In order to take advantage of the benefits of both methods, a coupled continuous/discontinuous approach, involving a continuum damage model in its integral-type nonlocal formulation and an extrinsic discrete interface model which is thermodynamically consistent, is proposed to model the complete failure process of quasi-static materials. The transition from diffuse damage to macroscopic crack is made through the equivalence of dissipated energy when the damage around the crack tip reaches a critical value. This approach is implemented in the extended finite element framework, exploiting the partition of unity property of shape functions which avoids remeshing during arbitrary crack propagation. Some benchmark problems are investigated to demonstrate the applicability and robustness of our method. Force-displacement curves, as well as the predicted propagation paths, are in close agreement with available experimental data. In addition, the effect of damage threshold for damage-crack transition is studied and consistent results are obtained for different threshold values.

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Title: A Computational Framework for the Simulation of High-Speed Multi-Material Fluid-Structure Interaction Problems with Dynamic Fracture

Author(s): Kevin Wang, *Virginia Tech*; Patrick Lea, Charbel Farhat, *Stanford U.*

A robust computational framework for the solution of Fluid-Structure Interaction (FSI) problems characterized by compressible flows and highly nonlinear structures undergoing pressure-induced dynamic fracture is presented. This framework is based on the Finite Volume method with Exact Riemann solvers (FIVER) for the solution of multi-material problems. It couples an Eulerian, finite volume based computational approach for solving flow problems with a Lagrangian, finite element based computational approach for solving structural dynamics and solid mechanics problems. Most importantly, it enforces the governing fluid-structure transmission conditions by solving local, one-dimensional, fluid-structure Riemann problems at evolving structural interfaces which are embedded in the fluid mesh. A generic, comprehensive, and yet effective approach for representing a fractured fluid-structure interface is also presented. This approach, which is applicable to several finite element based fracture methods including interelement fracture and remeshing techniques, is applied here to incorporate in the proposed framework two different and popular approaches for computational fracture in a seamless manner: the eXtended Finite Element Method (XFEM), and the Element Deletion (ED) method. Finally, the proposed embedded boundary computational framework for the solution of highly nonlinear FSI problems with dynamic fracture is demonstrated for one academic and three realistic applications characterized by detonations, shocks, large pressure and density jumps across material interfaces, dynamic fracture, flow seepage through narrow cracks, and structural fragmentation. Correlations with experimental results, when available, are also reported and discussed. For all four considered applications, the relative merits of XFEM and ED for computational fracture are also contrasted and discussed.

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Title: Towards High-Fidelity Design in the Age of Extreme-Scale Supercomputing

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

Extreme scale supercomputing will soon offer a million times the computing power of a desktop - an as drastic upgrade as that from a slide rule to a desktop computer in the 1990s. I believe this will revolutionize how engineers work. It will enable them to rapidly and confidently refine and optimize their designs. But this revolution can only happen through innovating computational algorithms. In Computational Fluid Dynamics, high-fidelity simulations such as Detached and Large Eddy Simulations can often reliably predict the performance of aerospace vehicles and engines. But with today's algorithms, these simulations take days if not weeks. With today's optimization algorithms, it may take months if not years for us to reach a good design. Can we shorten high fidelity optimization to minutes by innovating how we do optimization, again utilizing more concurrency than we currently can? I believe that the answer is yes. In this talk, I will show you why I believe so, and discuss a few promising research direction towards this goal, including the research area of parallel Bayesian optimization technique.

Title: Free Vibration Analysis of Thick Plates with Isogeometric Approach

Author(s): Wei Wang, Xiaoxiao Du, Gang Zhao, *Beihang U.*; Howie Fang, *U. North Carolina, Charlotte.*

The isogeometric method is used to study the free vibration of thick plates based on Mindlin theory. The Non-uniform Rational B-spline (NURBS) basis functions are employed to build the thick plate's geometry models and serve as the shape functions for solution field approximation in finite element analysis (FEA). This concept is referred to as Isogeometric Analysis (IGA) which was introduced by Hughes et al. in 2005 [1]. Various geometry-shapes containing square, circular and skew plates constructed by singular patch are considered and different essential boundary conditions such as clamped, simply supported and free boundary conditions are imposed on the boundaries of the plates. For the purpose of promoting the approach toward a more practical level, some complicated plate models represented by non-conforming multi-patches are also explored. In order to glue the non-conforming geometry patches, Nitsche method [2] is employed in the work. This method has two obvious advantages compared with mortar method and penalty method: firstly it keeps the size of equation system and secondly, maintains the positive definiteness of stiffness matrix. A stabilization parameter should be calculated by solving an eigenvalue problem to ensure the coercivity of the bilinear form. The mass matrices for each patch are assembled by using a lumped approach. The natural frequencies for different cases are obtained by solving the eigenvalue equation and compared with the existing reference solutions involving the results from element-free Galerkin method (EFG), generalized differential quadrature method (GDQ), etc. Graphs of various vibration mode shapes are plotted with the obtained eigen vectors for more intuitive demonstration. The results of numerical examples show the robustness, accuracy and high-efficiency convergence of the isogeometric analysis approach. Nitsche method provides us with a good approximation to non-conforming situations and relieves us from the pains-taking coupling operation for obtaining conforming mesh. It shows that the natural frequencies can be successfully predicted by the combination of isogeometric analysis and Nitsche method. [1]. 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. [2]. J. Nitsche. über ein variationsprinzip zur löung von dirichlet-problemen bei verwendung von teilräumen, die keinen randbedingungen unterworfen sind. *Abhandlungen aus dem mathematischen Seminar der Universität Hamburg*, 1971. 36: 9-15.

Title: Analytical and Numerical Study of a Simple A Posteriori Error Estimator for a Quasicontinuum Approximation

Author(s): Hao Wang, *Sichuan U.*; Mingjie Liao, *Beijing Sci. & Tech. U.*; Lei Zhang, *Shanghai Jiaotong U.*.

This presentation focuses on the analytical and numerical study of a simple a posteriori error estimator, whose construction is based on an averaging of the gradient, for a quasicontinuum approximation, which is the Geometrically Reconstructed Atomistic/Continuum Coupling Method (GR-AC method) that is recently developed. This simple error estimator was first employed in [1] for the adaptivity of the quasicontinuum method. Although the estimator is easily constructed and is widely used in practice, it has not received any analytical study to the best knowledge of the authors. Recent rigorous analysis has mainly focused on the residual based a posteriori error estimators [2,3]. However, the difficult implementation and the high computational cost of the estimator makes the residual based approach of only theoretical significance. The current research tries to bridge the gap between theory and practice. The presentation consists of four parts. In the first part, we briefly introduce the construction of the residual based a posteriori error estimator; In the second part, we show the efficiency of such estimator; In the third part, we prove that the simple estimator based on the averaging of the gradient is an efficient estimate of the residual based one; In the final part, we illustrate the validity of our analysis by certain numerical experiments. We believe this fundamental research on the rigorous analysis of the a posteriori error estimate will provide a significant assistance to the effective and efficient application of the quasicontinuum method. [1] V.B. Shenoy, R.Miller, E.B.Tadmor, D.Rodney, R.Phillips, M.Ortiz, An Adaptive Finite Element Approach to Atomic-scale Mechanics-the Quasicontinuum method, *Journal of the Mechanics and Physics of Solids*, 47, 1999 [2] C.Ortner and H.Wang, A Posteriori Error Control for a quasi-continuum Approximation of a Periodic Chain, *IMA J. Numer. Anal.*, 34(3), 2014 [3] H.Wang, M.Liao, P.Lin and L.Zhang, A Posteriori Error Estimate for Atomistic/Continuum Coupling in 2D, manuscript

Title: Isogeometric Fluid–Structure Interaction Analysis of Hydraulic Energy Absorbers

Author(s): Chenglong Wang, Ming-Chen Hsu, Yuri Bazilevs, *Iowa State U.*

The aim of this work is to simulate the fluid–structure interaction (FSI) of hydraulic energy absorbers. Hydraulic energy absorbers are widely used energy applications to transfer mechanical kinetic energy to hydraulic energy. An example of such application is the water twister used in an arresting gear system. The water-filled structure includes a rotating turbine (rotor) and a stationary reel (stator). To improve the efficiency of the CAD model construction, we propose a parametric modeling platform to generate analysis-suitable geometries for this complex system. Once the model is generated, we first perform CFD simulations at several rotational speeds using the finite element ALE–VMS formulation augmented with weakly enforced essential boundary conditions. The results are compared with the experimental data and excellent agreements were achieved. The sliding-interface method is adopted to handle the relative motion between the rotor and stator. We then simulate the FSI of the hydraulic energy absorber by applying the isogeometric Kirchhoff–Love thin shell theory to the rotor blades constructed using T-spline functions. The fluids and structures are coupled using a block-iterative approach. The FSI simulation results will be presented and discussed.

Title: Numerical Analysis of the Interaction Between Wave and Sandy Seabed with a New Constitutive Model

Author(s): Zhongtao Wang, Peng Liu, *Dalian U. Tech.*

The wave-induced liquefaction of seabed causes serious damage to offshore installations and structures. The constitutive behavior of sand is related to state-parameter-dependent dilatancy which depends on the current physical state such as void ratio and stress state like confining pressure. And the principal stress axes rotation is another important reason contributing to wave-induced seabed liquefaction and shear failure. Based on the generalized plasticity theory, a constitutive model for sand incorporating the effects of principal stress rotation and state-parameter-dependent dilatancy is proposed. And this proposed sand constitutive model has been included into the generalized finite element program DIANA-SWANDYNE II to simulate the wave-induced dynamic response of level seabed. The excess pore pressure generation due to the principal stress rotation has been investigated to validate the new constitutive model. From the results of the simulation, the proposed model is proven to have the ability of reflecting the effects of both principal stress rotation and state-parameter-dependent dilatancy for the analysis of the interaction of wave and sandy seabed. The conclusion provides technical support for the design of offshore engineering.

Title: Variationally Consistent Coupling of Non-Matching Finite-Element and Mesh-Free Discretizations

Author(s): Xiaowo Wang, Arun Prakash, *Purdue U.*

Numerical analysis of large-scale problems in structural mechanics that span multiple scales of response usually requires very fine spatial and temporal discretization. However, using a uniformly small size of time-step and fine mesh/discretization for the entire domain is computationally very expensive. Domain decomposition is an approach that allows one to reduce this computational cost by dividing the structure into smaller subdomains and using different levels and types of discretizations for different subdomains. However, various numerical issues arise in the process of coupling these subdomains back and enforcing continuity across the interfaces to obtain the global solution. By using different types of discretizations, such as meshfree methods and finite element methods, or by using different levels of finite element mesh refinement in adjacent subdomains, non-matching interfaces are created. Models containing such non-matching interfaces are in general not able to pass basic patch test due to inconsistencies in the numerical integration across these interfaces. In this study, a variationally consistent coupling (VCC) method is developed to ensure that basic patch tests are passed by models containing non-matching interfaces for any choice of numerical integration over the interface. In addition to non-matching meshes in space, the use of different time steps in different subdomains can also lead to problems. A simplified multi-time-step coupling method for non-linear problems is presented which possesses improved computational efficiency over the conventional consistent multi-time-step method. Numerical examples investigating both these aspects domain decomposition, spatial and temporal, are presented to study the performance of the proposed methods and to study the effect of the presence of these numerical interfaces in such coupled models.

Title: Generalizations of Randomize-Then-Optimize (RTO): Optimization-Based Sampling Algorithms for Bayesian Inference

Author(s): Zheng Wang, Youssef Marzouk, *MIT*.

In the Bayesian statistical paradigm, uncertainty in the parameters of a physical system is characterized by a probability distribution. Information from observations is incorporated by updating this distribution from prior to posterior. Quantities of interest, such as credible regions, event probabilities, and other expectations can then be obtained from the posterior distribution. One major task in Bayesian inference is then to characterize the posterior distribution, for example, through sampling. Markov chain Monte Carlo (MCMC) algorithms are often used to sample from posterior distributions using only unnormalized evaluations of the posterior density. However, high dimensional Bayesian inference problems are challenging for MCMC-type sampling algorithms, because accurate proposal distributions are needed in order for the sampling to be efficient. [1] presents an alternative optimization-based algorithm to obtain efficient proposals, called 'Randomize-then-Optimize' (RTO). Other optimization-based sampling schemes include implicit sampling [2], randomized maximum likelihood, and variants of optimal maps [3]. We build upon the sampling algorithm presented in [1] by developing a new geometric interpretation that describes RTO samples as projections of Gaussian-distributed points, in the joint data and parameter space, onto a nonlinear manifold described by the forward model. This interpretation reveals generalizations of RTO that can be used to make it more efficient. We also draw connections between RTO and implicit sampling [2], as well as inference approaches using transport maps [3]. Finally, we introduce a variable transformation that generalizes RTO to problems with non-Gaussian priors, such as Bayesian inverse problems with Besov space priors. We demonstrate significant computational savings from this strategy on a high-dimensional inverse problem. References: [1] Bardsley, J. M., Solonen, A., Haario, H., and Laine, M. (2014). Randomize-then-optimize: a method for sampling from posterior distributions in nonlinear inverse problems. *SIAM Journal on Scientific Computing*, 36(4): A1895–A1910. [2] Morzfeld, M., Tu, X., Atkins, E., and Chorin, A. J. (2011). A random map implementation of implicit filters. *Journal of Computational Physics*, 231: 2049–2066. [3] Parno, M. and Marzouk, Y. M. (2014). Transport map accelerated Markov chain Monte Carlo. *arXiv:1412.5492*.

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Title: Understanding and Modeling Nucleation, Growth, and Interaction of Deformation Twins in Hexagonal Materials

Author(s): Jian Wang, *Los Alamos Nat'l. Lab.*

Deformation twinning is a major mode of plastic deformation in hexagonal-close-packed crystals and exhibits more complex nucleation and propagation mechanisms than those in cubic structure. In this lecture, I highlighted several twinning-associated boundaries that play crucial roles in nucleation, growth, and interactions of deformation twins in hcp metals. According to microscopic characterizations and atomistic simulations, nucleation mechanisms, propagation and growth mechanisms, and interactions of deformation twins are discussed. Four types of boundaries related to these events are reviewed including (1) symmetrical tile grain boundaries (SCTGs) that favor twin nucleation or migrate based on twin dislocations, (2) prismatic-basal boundaries (PBs or BPs) associated with twin nucleation via pure-shuffle mechanism, (3) serrated coherent twin boundaries (SCTBs) associated with migration of twin boundaries via glide and climb of twinning dislocations, and (4) prismatic-prismatic (PPs) and basal-basal (BBs) boundaries associated with co-zone twin-twin interactions. More importantly, these boundaries affect twinning and detwinning processes that may correspond to twinning-induced hardening and seem universal associated with twins in hexagonal-close-packed metals. These findings provide theoretical base for researchers to revisit experimental data, rebuild the frame of twinning mechanisms including nucleation and propagation of twins, and advance the development of materials modeling tools at meso- and macro- scales as well as alloy design.

Title: Non-Linear, Finite-Element Analysis of Partially-Saturated Fractured Porous Media Using a Coupled Thermo-Poro-Mechanical Cohesive Interface Element

Author(s): Wei Wang, *LLNL*; Richard Regueiro, *U. Colorado-Boulder*.

The coupling between multiphase flow, heat transfer, and poromechanics in fractured geomaterials has aroused great interest in the areas of geomechanics, geoenvironmental engineering, and petroleum engineering. Relevant applications include nuclear waste repositories, geological sequestration of CO₂, geothermal systems, and exploitation of shale gas reservoirs. Based on porous media theory, the authors propose a fully coupled thermo-poro-mechanical (TPM) cohesive interface element (CIE) model, which can represent multiphase flow and heat transfer within and across pre-existing discontinuities. Including an appropriate constitutive model for the effective traction at the interface can capture the propagation of discontinuities. The solid skeleton of the matrix (or bulk rock) is assumed to be pressure-sensitive nonlinear isotropic elastic. A traction-displacement model is adopted to represent shear/normal deformation along the discontinuity. The system of tightly coupled equations is solved monolithically for four primary variables, i.e. pore water and pore gas pressures, rock mixture temperature, and solid skeleton displacement within the bulk continuum and also jumps along the discontinuities. To explore an efficient, yet accurate and stable finite element solution for the nonlinear matrix equations, two essential ingredients (time integration scheme and element type) are considered through several numerical examples. In terms of time integration scheme, a fully-implicit method using the Newon-Raphson algorithm is shown to be more stable and accurate for larger time steps, yet slower computationally than the semi-implicit schemes (conditionally stable) which lead to linear solution at each time step. In addition, a comparison is made between various combinations of mixed finite elements: (i) Q4P4/Q4P4S for both bulk and interface elements; (ii) Q9P4 for bulk elements and Q6P4 for interface elements.

Title: Proportional Topology Optimization Method for Frequency Optimization of 3D Printed Components

Author(s): Xue Wang, Emre Biyikli, Albert C To, *U. Pittsburgh.*

Frequency optimization has an important role in engineering structures to avoid resonance. This paper introduces a new topology optimization method called the Proportional Topology Optimization (PTO) [1] that maximizes the minimum natural frequency in the system in order to keep the resonant frequency away from external excitation frequency range. PTO is a non-sensitivity algorithm that aims to solve the difficulties associated with sensitivity-based methods. A common problem in frequency optimization is that localized modes emerge in areas with lower densities. Standard approaches like the SIMP [2] does not resolve the issue. Therefore, a new polynomial interpolation function [3] is utilized to penalize the Young's modulus. Several numerical examples are presented. Results show that the PTO method maximizes the minimum natural frequency of structures and reaches to a black/white solution. The polynomial interpolation penalization successfully avoids localized modes. The method will be applied to optimize several structures and the optimized structures are realized by 3D printing. References: [1] Emre Biyikli, and Albert C. To (2014). Proportional Topology Optimization: A new non-sensitivity method for solving stress constrained and minimum compliance problems and its implementation in MATLAB, under review. [2] Niels Leergaard Pedersen (2000). Maximization of eigenvalues using topology optimization. *Struct Multidiscip Optimiz.*20:2-11. [3] Bin Wang (2010). Multi-performance optimization of structures and its application in aerospace structural design. Ph.D. Thesis. Dalian university of technology.

Title: Quasi-Convex Reproducing Kernel Meshfree Approximants

Author(s): Dongdong Wang, Pengjie Chen, Hanjie Zhang, Junchao Wu, *Xiamen U., Fujian* .

Convex meshfree approximations are very desirable due to their sound solution accuracy, particularly for structural vibration analysis. However, the commonly used moving least square or reproducing kernel meshfree shape functions are not convex approximations. In this paper, a new quasi-convex reproducing kernel approximation scheme is developed for meshfree analysis. The present quasi-convex reproducing kernel meshfree approximants are designed under the umbrella of the relaxed reproducing or consistency conditions which are almost identical to the classical consistency conditions, thus the shape functions of the proposed meshfree approximants have a similar form as their reproducing kernel counterparts. As a result, the proposed scheme can be conveniently implemented in the standard reproducing kernel meshfree formulation without extra computational effort. Meanwhile, the present formulation enables a straightforward construction of arbitrary higher order shape functions. It is shown that the proposed method yields nearly positive shape functions in the interior problem domain, while in the boundary region the negative effect of the shape functions are also reduced compared with the original reproducing kernel meshfree shape functions. It is also shown that the derivatives of the proposed quasi-convex reproducing kernel meshfree shape functions are more smoothing than those of the traditional reproducing kernel shape functions. Thereafter a Galerkin meshfree analysis is systematically performed by employing the proposed quasi-convex reproducing kernel shape functions. Both the 2nd order problems such as 1D rod, 2D membrane and elasticity problems, and the 4th order problems of thin beams and plates are studied to assess the performance of the present method. Numerical results demonstrate that the proposed method have more favorable accuracy than the conventional reproducing kernel meshfree method. Acknowledgements: The support of this work by the National Natural Science Foundation of China (11222221, 11472233) and the Natural Science Foundation of Fujian Province of China (2014J06001) is gratefully acknowledged.

Title: Weighted ℓ_1 Minimization for High-Dimensional Function Approximation

Author(s): Rachel Ward, *UT Austin*.

Functions of interest are often smooth and sparse in some sense, and both priors should be taken into account when interpolating sampled data. Classical linear interpolation methods are effective under strong regularity assumptions, but cannot incorporate nonlinear sparsity structure. At the same time, nonlinear methods such as ℓ_1 minimization can reconstruct sparse functions from very few samples, but do not necessarily encourage smoothness. Here we show that weighted ℓ_1 minimization effectively merges the two approaches, promoting both sparsity and smoothness in reconstruction. More precisely, we provide specific choices of weights in the ℓ_1 objective to achieve rates for functions with coefficient sequences in weighted ℓ_p spaces, $p \leq 1$. We consider the implications of these results for spherical harmonic and polynomial interpolation, in the univariate and multivariate setting. Along the way, we extend concepts from compressive sensing such as the restricted isometry property and null space property to accommodate weighted sparse expansions; these developments should be of independent interest in the study of structured sparse approximations and continuous-time compressive sensing problems. This is joint work with Holger Rauhut (Aachen University).

Title: The Dynamics of Error and Rate of Convergence for High-Order Flux Reconstruction

Author(s): Jerry Watkins, Kartikey Asthana, Antony Jameson, *Stanford U.*

Among high-order methods, the Flux Reconstruction (FR) approach has proved to be a simple and useful tool in solving hyperbolic equations. The framework allows for the recovery of a variety of different schemes including Discontinuous Galerkin (DG) and spectral difference (SD) methods while maintaining features from finite volume methods. Huynh offers an insight into the stability and accuracy of specific schemes under FR but the numerical properties of the method have yet to be completely analyzed [1]. This presentation hopes to clarify the dynamic aspects of order of accuracy and formulate a consistency proof for high-order FR. Using Fourier analysis, the semi-discrete FR equation is formulated from the 1D linear scalar conservation law. The exact solution of the linear dynamical system forms one physical mode followed by P spurious modes where P is the polynomial order of the scheme. The characteristic time scales associated with the spurious modes are small and dissipate very quickly. As the spurious modes dissipate, energy is lost and the error associated with this loss lingers in the solution. After the spurious modes dissipate, the physical mode dominates and accuracy of the scheme is dictated by the physical mode and error associated with numerical differentiation. The dynamics of error give a clear explanation of the evolution of the rate of convergence. An error evolution equation is formulated and a forcing term associated with numerical differentiation error emerges. For small time, this error dictates the accuracy of the solution. A number of theorems are proven including: The forcing term is at least $(P+1)$ order accurate for any flux, correction function or choice of solution point. After a long time, the error associated with the physical mode dominates due to dissipation in the physical mode. This error dictates the accuracy of the solution and can be found by defining a relative error which eliminates the error associated with numerical differentiation. The order of accuracy is found by performing a series expansion of the eigenvalue associated with the physical mode and a number of theorems can be formulated for low polynomial orders. [1] Huynh, H. T. "A flux reconstruction approach to high-order schemes including discontinuous Galerkin methods." AIAA paper 4079 (2007): 2007.

Title: Topology Design in Inverse Homogenization for Thermoelastic Properties

Author(s): Seth Watts, Daniel Tortorelli, *U. Illinois*; Christopher Spadaccini, *LLNL*.

The development of new techniques in additive micro-manufacturing in recent years has enabled the fabrication of material microstructures with essentially arbitrary designs, including those with multiple constituent materials and void space in nearly any geometry. With an essentially open design space, the onus is now on the engineer to design composite materials which are optimal for their purpose. These new materials, called meta-materials or materials with architected microstructures, offer the potential to mix and match properties in a way that exceeds that of traditional composites. We concentrate on the thermal and elastic properties of isotropic meta-materials, and design microstructures with combinations of Young's modulus, Poisson's ratio, thermal conductivity, thermal expansion, and mass density which are not found among naturally-occurring or traditional composite materials. We also produce designs with thermal expansion far below other materials. We use homogenization theory to predict the material properties of a bulk meta-material comprised of a periodic lattice of unit cells, then use topology optimization to rearrange two constituent materials and void space within the unit cell in order to extremize an objective function which yields the combinations of properties we seek. This method is quite general and can be extended to consider additional properties of interest. We constrain the design space to satisfy material isotropy directly (2D), or to satisfy cubic symmetry (3D), from which point an isotropy constraint function is easily applied. We develop and use filtering, nonlinear interpolation, and thresholding methods to render the design problem well-posed and to ensure our designs are manufacturable. We have written two computer implementations of this design methodology. The first is for creating two-dimensional designs, which can run on a serial computer in approximately half an hour. The second is a parallel implementation to allow optimization in three dimensions with a large number of parameters. When running on a high-performance computing cluster, it allows for solutions in a few hours despite the greatly increased computational cost.

Title: Numerical Modeling of a Glass Curtain Wall Subjected to Low-Level Blast Loads

Author(s): Adam Ralston, *Little Diversified Architectural Consulting*; David Weggel, Matthew Whelan, Howie Fang, *UNC Charlotte*.

Glass curtain walls are common façade elements in modern commercial construction. Traditionally they have been designed to resist wind loads and to accommodate building drift. However, it is becoming more common to design glass curtain walls to resist some level of blast loading, especially if the building is perceived to be the target of a terrorist attack or could suffer collateral damage by being in close proximity to a more likely target. This paper describes the development of the simplest adequate finite element model of a glass curtain wall suitable for general blast loading analysis. The modeled curtain wall is one-way, vertically spanning and has conventional hardware and aluminum extrusions for its frame (mullions) as well as laminated glass lites that are adhered to the frame with structural silicone sealant. The model has been validated with test results from a series of full-scale curtain wall specimens subjected to low-level blast loads. FE simulations with this validated model captured the complex responses of the curtain wall system, which included glass cracking and tearing of silicone sealant. While the model could accommodate yielding of the aluminum mullions, the blast loads were small enough such that no yielding resulted. Simulation times of 0.1s required approximately two hours of computational time using 32 compute cores. Simulation results indicated the importance of accounting for negative-phase blast pressures (pressures below ambient pressure), in addition to positive-phase pressures. Further, total damping – comprised of structural damping, aerodynamic damping, and fluid-structure interaction damping – must be carefully considered for the simulation results to compare well with test results. The best FE model produced nonlinear dynamic deflections of glass lites and mullions that agreed well with the test results. Glass cracking patterns and tearing of the structural silicone sealant were generally representative of the test results.

Title: Response of Biopolymer Networks Governed by the Physical Properties of the Cross-Linking Molecules

Author(s): Xi Wei, Yuan Lin, *U. Hong Kong*; Vivek B. Shenoy, *U. Pennsylvania*.

It is well-known that the mechanical response of live cells is largely determined by its cytoskeleton, a network consisting of different bio-filaments such as F-actin and microtubules that are interconnected and bundled together by a variety of crosslinking proteins. Although accumulating evidence has shown that the physical properties of cross-linkers can significantly influence the bulk behavior of such biopolymer networks, the underlying mechanisms remain unclear and a quantitative mapping between the two is still lacking. Here we present a computational study to address this important issue. Specifically, a combined finite element – Langevin dynamics (FEM-LD) approach was employed to examine the mechanical behavior of randomly cross-linked F-actin network where, besides bending and stretching, thermal fluctuations of individual filament have also been taken into account. The cross-linker is modeled as a combination of linear and rotational springs that resists both separation and relative rotation between two filaments and disengages from the F-actin once the strain energy stored inside reaches a critical level. It was found that networks with compliant cross-linkers exhibit low bulk moduli with no apparent strain-hardening because most of the imposed strain was actually absorbed by those highly-deformable crosslinking molecules. In addition, we showed that increasing the rotational spring stiffness of cross-linkers will lead to a more homogeneous load distribution, as well as deformation, within the network. Interestingly, stress-strain curves obtained from our simulations are decorated with sudden load drops, corresponding to the breakage of individual crosslink points, which demonstrates that deformation will generally not progress in a smooth fashion. Finally, the influence of entropy was found to be important only when the strain level is low (less than ~1%) while the network response is dominated by elasticity at large strains. Nevertheless, thermal fluctuations of F-actin seem to always advance the onset of crosslink breakage. Connections between our results and various experimental findings will also be discussed.

Title: Truncated T-Splines

Author(s): Xiaodong Wei, Yongjie Zhang, *Carnegie Mellon U.*

In this talk, we present a new method termed Truncated T-splines, which support local refinement without propagation. Unlike traditional T-splines, truncated T-splines do not require edge extension, and thus the refinement of truncated T-splines does not propagate beyond the region of interest. This is benefited from the truncation mechanism of underlying T-spline basis functions. Moreover, truncated T-splines exactly preserve the geometry during local refinement. From the viewpoint of geometric design, truncated T-splines are advantageous in handling control meshes of arbitrary topology, which is also a property inherited from T-splines. Truncated T-spline basis functions are polynomials and satisfy partition of unity, which ensures the convex hull property. From the viewpoint of analysis, Truncated T-splines produce linearly independent basis functions and they are also proved to successfully pass the patch test in regular and irregular control meshes. Therefore, the truncated T-spline is suitable for both geometric design and analysis, which makes it a promising candidate for isogeometric analysis. Several examples are used to demonstrate the proposed method.

Title: Towards a Stabilized Meshfree Formulation for Hydraulic Fracturing Simulation

Author(s): Haoyan Wei, J. S. Chen, *UC San Diego*.

Numerical modeling of low permeable reservoirs often suffers from spurious fluid pressure oscillations due to violation of the inf-sup condition. Such difficulty must be overcome for a robust hydraulic fracturing simulator since the permeability of shale is extremely low. To this end, a stabilized meshfree formulation is developed based on a fluid pressure projection method, in which an additional stabilization term is added to the variational equation to correct the deficiency of the equal-order u-p approximation. Within this framework, an L2 projection operator is defined locally inside a representative domain of each node. It is shown that the projection scheme is compatible with the stabilized conforming nodal integration which enables a significant enhancement of the computational efficiency, and thus these two methods are naturally integrated into a unified framework where spurious low-energy modes of nodal integration are also eliminated. Several benchmark problems are analyzed to demonstrate the effectiveness of the proposed stabilized meshfree formulation. The proposed method in conjunction with the implicit gradient regularization method is then extended to model hydromechanical fracture and damage (smeared cracks) processes in fracking.

Title: Locking-Free Pyramid Finite Elements for Transitional Mesh

Author(s): Ravi Burla, David Weinberg, Jaesung Eom, *Autodesk Inc.*.

Automatic mesh generation for complex geometries is desirable for analyzing many physical systems with Finite Element Method. Hexahedral mesh is preferred for various analysis types, however generating a mesh automatically with all hexahedral elements is difficult and most industrial FEA packages use hex dominant meshes. A hex-dominant mesh often leads to wedge, pyramid and tetrahedral transitional elements. In this work, pyramid transition elements are proposed. B-Bar approach is used to overcome volumetric locking in linear pyramid elements. Linear (5-noded) and Quadratic (13-noded) pyramid elements shape functions are constructed based on the corresponding hexahedral element shape functions. Integration of stiffness matrices is performed using hexahedral-like quadrature rules. The element is applied to several different analysis types – (a) Linear Static Stress (b) Modal (c) Linear and nonlinear heat transfer (d) Nonlinear quasi-static analysis with large deformations. The element is also extended for nonlinear materials – (a) Hyperelastic, (b) Elastic Plastic. Several numerical examples are studied to evaluate the performance of pyramid elements. Results are compared and contrasted with hexahedral and tetrahedral elements. Linear pyramid element undergoes volumetric locking for near incompressible materials. Strain projection (B-Bar) approach [1] is used to overcome the locking. In this approach, strain-displacement (B) matrix is split into dilatational (B_{dil}) and deviatoric (B_{dev}) components. The dilatational component (B_{dil}) is updated by improved dilatational contribution ($B\bar{B}_{dil}$). Two approaches are used for computing $B\bar{B}_{dil}$ (a) Element centroidal value of B_{dil} is used for $B\bar{B}_{dil}$, (b) Volumetric mean of B_{dil} over element volume is used for $B\bar{B}_{dil}$. Numerical examples are provided to demonstrate the suitability of this approach for the pyramid elements. [1] Hughes T.J.R., 2000. The Finite Element Method: Linear Static and Dynamic Finite Element Analysis. Dover Publications, New York.

Title: The Fast Directional Algorithm Accelerated Topological Sensitivity Analysis for Acoustic Inverse Problems

Author(s): Lihua Wen, Yanchuang Cao, Jinyou Xiao, *Northwestern Polytech. U.*

Identifying the obstacles in acoustic fields plays important roles in many engineering problems, such as acoustic imaging, sonar designing, etc. The topological sensitivity analysis is believed as one of the promising methods for these acoustic inverse problems, in which the topological derivatives of the cost function are used as an indicator for the obstacles location. The pressure and velocity fields of two acoustic forward problems have to be solved to evaluate the topological derivatives. In this work, they are solved efficiently by method of fundamental solutions (MFS), and it is accelerated by a wideband kernel independent fast algorithm, namely the fast directional algorithm (FDA). No integral is required in MFS, thus the entries of the resulting system matrix are just the kernel evaluations. Consequently, our fast method is completely kernel independent and easy to implement. Although the pressure and velocity fields are evaluated by different kernels, most of the translation matrices can be the same, thus these matrices are computed only once and shared in the evaluations of both fields. The almost optimal computational complexity and high convergence rate of the FDA accelerated MFS are demonstrated by numerical examples. The application in the topological sensitivity analysis shows that our method can identify the obstacles effectively and efficiently.

Title: On a Multi-Scale and Multi-Phase Model for the Description of Liver Perfusion and Metabolism

Author(s): Tim Ricken, Daniel Werner, *TU Dortmund U.*; Hermann-Georg Holzhütter, Matthias König, *Charite*; Uta Dahmen, Olaf Dirsch, *U. Clinic of Jena*.

Metabolism in the liver is a complex multi-phase, multi-scale, time depending and non-linear coupled function-perfusion-mechanism. The function of the liver, e.g. nutrient storage and uptake of drugs, is directly coupled to its blood perfusion. In this talk we present a computational model that describes selected coupled functionalities. The metabolic processes take place in the liver cells, the hepatocytes, which are arranged in hexagonal functional segments, the liver lobules. Nutrients, oxygen, and other components of the blood are transported to the hepatocytes through a delicate system of capillaries, so called sinusoids. The inhomogeneous distribution of the sinusoidal network leads to an anisotropic blood flow in the liver lobules. Due to this highly complex inner structure of the lobules it is impracticable to give a microscopic geometrical description in a continuum mechanical manner. Therefore, a homogenization scheme based on the mixture theory, the so called theory of porous media (TPM), is used; see [1]. In case of the presented liver model we consider a porous solid body and a fluid. Both phases are considered as immiscible, heterogeneously composed materials. Each phase contains one carrier phase and several miscible components. The solid carrier phase contains a set of internal concentrations, such as glycogen and triglyceride, whereas the fluid carrier phase contains a set of external concentrations, such as glucose and lactate. For the microscopic cell level use of an embedded set of ordinary differential equations (ODE) is made. The ODE model mimics a simplified metabolism that takes place in the hepatocytes converting nutrients into vital products, such as glucose. Knowledge of glucose production, utilization, and storage is a necessity for the description of fat accumulations within the liver; see [2]. REFERENCES [1] de Boer, R.: Theory of Porous Media. Springer-Verlag, Berlin 2000. [2] Ricken, T. et al. Modeling function-perfusion behavior in liver lobules including tissue, blood, glucose, lactate and glycogen by use of a coupled two-scale PDE-ODE approach. Biomechanics and Modeling in Mechanobiology, 1-22, doi:10.1007/s10237-014-0619-z (2014).

Title: A Multi-Dimensional Discontinuous Galerkin Modeling Framework for Overland Flow

Author(s): Dustin West, Ethan Kubatko, *Ohio State U.*

We present the development and application of a multidimensional (2-D & 1-D) kinematic wave model in a discontinuous Galerkin framework for simulating overland flow and runoff due to torrential rainfall. The purpose of this work is to improve on (1) the modeling approach involving many small-scale rivers and channels and (2) the accuracy of flooding caused by storm surge coupled with torrential rainfall. The overland flow is modeled using the 2-D kinematic wave equations derived from the 2-D depth averaged shallow water equations. In areas of the domain where flow converges into channels, the edges of 2-D elements are used as 1-D channels for flow routing. To best represent complex topography, domains are discretized using an application developed by the authors called Admesh+ [1], an automatic unstructured mesh generator for shallow water models. Admesh+ produces high-quality meshes with the appropriate amount of refinement where it is needed to resolve all of the geometry and flow characteristics of the domain. The mesh generation technique utilizes high-resolution digital elevation maps (DEMs) to automatically produce unstructured meshes with elements arranged to best represent shorelines, channel networks and watershed delineations. The development of the multidimensional overland flow model and mesh generation techniques are presented along with comparisons of model results with various analytic solutions and experimental data. [1] Colton J. Conroy, Ethan J. Kubatko, DustinW.West. "ADMESH: An advanced unstructured mesh generator for shallow water models",. Ocean Dynamics, December 2012, Volume 62, Issue 10-12, pp 1503-1517.

Title: Numerical Modeling of Cold-Formed Steel Stud Walls with Conventional Stud-to-Track Connections Subjected to Blast Loads

Author(s): Michael Connor, Matthew Whelan, David Weggel, *U. North Carolina-Charlotte*; Adam Ralston, *Little Diversified Architectural Consulting*.

Cold-formed steel stud walls are a conventional structural component used for expedient construction of both civilian and military buildings. If properly detailed, these walls offer good resistance to blast loads through a combination of high strength and ductility that enables dissipation of blast energy through large deformation kinematics. However, achieving the full tension membrane resistance in conventionally-constructed steel stud walls is often precluded by limit states associated with the stud-to-track connections. Furthermore, the presence of local and distortional buckling modes associated with the thin-walled, open cross-section of conventional studs provides additional challenges with respect to dynamic analysis. Consequently, understanding the response of cold-formed steel stud walls in the region of response between yielding and full tension membrane resistance through both testing and extended numerical analyses is paramount to the design of these systems when considering protective measures, even for resisting low-level blast loads. This presentation describes the development and experimental verification of a high-fidelity finite element model of a cold-formed steel stud wall subjected to blast overpressures resulting from the detonation of a close-in charge. The model parallels specimens from an open arena blast program, where the performance of one-way spanning wall panels comprised of four studs with a bridging system and sheathing was examined. These wall specimens featured conventional stud-to-track connections with the base of each stud connected to the supporting track through a screwed connection, while the top of each stud featured a clip connection that allowed for vertical deflections and therefore prevented any axial load transfer into the studs. Details related to modeling cold-formed steel stud walls with these conventional connections for blast load analysis are presented with comparisons to blast test results. Initial verification of the model is provided through comparison of linear modal parameters with those estimated through experimental modal analysis of the specimens performed prior to blast testing. Subsequently, the model is used to predict the dynamic response and failure modes of the wall under the blast loading applied in the tests, and comparisons are made to the dynamic displacements recorded during the blast event. Lastly, permanent-set deformations measured through structured light scanning of the specimens is used to assess the model correlation with observed failure modes in the studs and stud-to-track connections.

Title: Adjoint-Based a Posteriori Error Estimation and Uncertainty Quantification for Shock-Hydrodynamic Applications

Author(s): Tim Wildey, John Shadid, Eric Cyr, *Sandia Nat'l. Lab.*

While adjoint-based error estimation is a well-established approach to quantify the global affect of local discretization errors on quantities of interest for numerical approximations of a variety of physical systems, the literature on adjoint methods for shock-hydrodynamic applications is actually rather sparse and recent. Early investigations with continuous adjoint formulations required accurate knowledge of the location of the discontinuities, which is infeasible for realistic applications. Recent work has shown that considering an alternative dual problem based on the concept of limiting viscosity may mitigate this issue. We compare and evaluate this approach using both discontinuous Galerkin approximations and weighted essentially non-oscillatory (WENO) approximations for shock-hydrodynamic applications. More recently, adjoint-based methods have proven quite useful in estimating the error in (and adaptively resolving) response surface approximations for quantities of interest computed from PDEs with uncertain parameters. The main difficulty in constructing response surface approximations for shock-hydrodynamics problems is the fact that the response surface may, and likely will, have discontinuities due to the presence of shocks. Several approaches have been developed to adaptively resolve the discontinuity including adaptive sparse grids, adaptive simplices methods, and adaptive voronoi-based approximations. We show how adjoint-based information, namely, derivatives of the quantity of interest with respect to the parameters, can be used to detect discontinuities and to adapt the response surface approximation and resolve the discontinuity. Unfortunately, the computational resources required to adaptively resolve the discontinuity often exceed those needed to accurately compute the statistics using standard methods. To mitigate this difficulty, we present an approach to robustly bound the error in the statistics computed from a response surface approximation with discontinuities that does not require that we resolve the discontinuity.

Title: Dielectric Breakdown Modeling Using Peridynamics

Author(s): Raymond Wildman, George Gazonas, *US Army Rsch. Lab.*

Dielectric breakdown is a phenomenon that occurs when a solid material is subjected to high voltage or electric field. Fracture of the material occurs through a complicated interaction between several fields, including electric, thermal, and mechanical. In this work, a multiphysics-based model of dielectric breakdown is constructed using peridynamics to model the mechanical failure of a material. In addition, thermal and electrostatic coupling is considered in the constitutive response. A basic summary of the process is as follows: A high voltage or field is applied to a material producing electrostatic forces that are felt by the material from both the Lorentz force and the Kelvin polarization force. In addition, a rise in temperature is seen due to Joule heating which affects other material properties. Specifically, electrical conductivity is coupled with both temperature and electric field, and permittivity is coupled with mechanical damage. Material parameters are coupled in such a way as to generate competing negative and positive feedback paths, leading to a complex, nonlinear process. Numerically, the mechanical fields are computed using peridynamics, a non-local method used in fracture analysis. A standard, point-based discretization is used. The electrostatic fields are computed using a finite difference method. The finite difference method uses a staggered grid, so that the electric potential is solved at grid points a half-step offset from the material properties and other fields. This approach is useful as the required forces are derived from the electric field, which is related to the gradient of the electric potential. Diffusion is not considered for the thermal fields, due to the short time scales and low thermal conductivities of the materials involved. Instead, thermal build-up is considered so that the change in temperature is related to the power generated by Joule heating. Results show that complex branching patterns can be generated even without explicitly including probabilistic tree growth as with other methods, such as the dielectric breakdown model. Random variation in the conductivity can be added to generate even more complex breakdown patterns.

Title: Error Analysis of DIC Imaging Data Using Least Square Approximation

Author(s): Shahriyar Beizaei, Kaspar Willam, *U. Houston*; Giovanna Xotta, *U. Padova*.

In the field of experimental solid mechanics, conventional strain measurement devices such as LVDT and strain gauges provide mean values of strains and displacements at selected locations and gauge lengths; this result is inadequate for the evaluation of a non homogeneous material behaviour. Consequently, during the last decades various full-field non-contact measurement techniques have been proposed for the material characterization and have become popular in the experimental mechanics community. In this work, the Digital Image Correlation (DIC) non-interferometric technique [1] has been used to monitor experiments on aluminum flat bars and to measure displacement distribution on the surface of the specimen for further evaluation and calculation of strains. The ARAMIS DIC-3D software by GOM has been adopted to process the measurements, to automatically compute the strains and to perform post-processing on the results. The results obtained by DIC are assessed and the error associated with the post processing of the experimental field data, obtained through the use of ARAMIS, is evaluated and analysed with the aid of a least square approximation code. This code uses a finite element approximation of the displacement field in order to cover all the target points. A least square approximation of these data is performed and the best nodal displacement values are determined. Based on the nodal data, infinitesimal and finite strain distributions are determined over the surface image window of the specimen and, using the strain data of the finite element approximation of the DIC data, the onset of failure and fracture is studied, coming up with appropriate methodologies to detect localization features on the specimen surface [2]. This can be achieved in several ways. One way is to calculate the vorticity, shear and divergence distribution on the surface of the specimen and locate discontinuous deformation features. Another way is to calculate the strain rate from one stage of imaging to another stage and to track the rank of the field of strain rate field by eigenvalue analysis. If there emerges a loss of rank, this indicates a jump in the strain rates and therefore loss of ellipticity or formation of weak discontinuities at the material level of observation. [1] Peters W.H., Ranson W.F. (1982), "Digital Imaging Techniques in Experimental Stress Analysis", Opt. Eng., 21(3), pp. 427-431. [2] Beizaei S. (2013), " Constitutive modelling and numerical implementation of brittle and ductile material behavior with the aid of inelastic XFEM and damage-plasticity models", PhD Thesis.

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Title: Computational Enhancements to Bayesian Design of Experiments Using Gaussian Processes

Author(s): Brian Williams, Brian Weaver, Christine Anderson-Cook, Dave Higdon, *Los Alamos Nat'l. Lab.*

Bayesian design of experiments is a methodology for incorporating prior information into the design phase of an experiment. Unfortunately, the typical Bayesian approach to designing experiments is both numerically and analytically intractable without additional assumptions or approximations. In this talk we discuss how Gaussian processes can be used to help alleviate the numerical issues associated with Bayesian design of experiments. We provide examples drawn from accelerated life testing and probabilistic calibration of model parameters and compare our results with large sample methods.

Title: Variationally Consistent Quadratic Finite Element Formulations for Contact Problems on Rough Surfaces

Author(s): Saskia Sitzmann, Kai Willner, *FAU Erlangen-Nuremberg*; Barbara Wohlmuth, *TU Munich*.

Although a lot of progress has been made in the implementation of contact algorithms in commercial codes, solving non-linear contact problems within the FEM framework is still a challenging task when facing large plastic deformations, non-linear material laws and several parts in contact in industrial applications. While suitable Lagrange multiplier based formulations are well-known for their consistency and stability in the case of classical model problems of Coulomb type, rough surface contact laws and additional multi-point constraints are much less understood. Especially for use in structural mechanics, it is often essential to model the asperities in the micro scale in order to reproduce measured behaviour like for example frictional damping. Instead of resolving the surface roughness on the micro scale in the FE discretisation, here the deformation of the contacting asperities is considered in a constitutive contact law resulting in regularized contact conditions. Additionally we focus on a quadratic approach avoiding numerical artefacts like shear locking, volumetric locking and hour-glassing and extend ideas from our previous work on constitutive contact laws [1, 2]. The popular dual mortar method is used to enforce the contact constraints in a variationally consistent way without increasing the algebraic system size [3]. To avoid possible consistency errors of the dual mortar approach in case of large curvatures in the contact zone leading to a physically incorrect evaluation of the dual gap, the Petrov-Galerkin mortar approach for linear elements is extended to the quadratic case. Moreover an adoption of the Lagrange Multiplier formulation being able to deal with directional blocking, cyclic symmetry and other multi point constraints as well as hanging nodes in the contact zone is presented bridging the gap to complex industrial applications. Numerical examples demonstrate the robustness of the derived numerical algorithm. Special focus is set to industrial motivated applications involving large deformations and plastic effects as well as rough surfaces on the micro scale. References [1] S. Sitzmann, K. Willner, B. I. Wohlmuth. A dual Lagrange method for contact problems with regularized contact conditions. *International Journal for Numerical Methods in Engineering* 99 (3): 221-238, 2014. [2] S. Sitzmann, K. Willner, B. I. Wohlmuth. A dual Lagrange method for contact problems with regularized frictional contact conditions: Modelling micro slip. *Computer Methods in Applied Mechanics and Engineering* 285 (0): 468-487, 2015. [3] B. I. Wohlmuth. A Mortar Finite Element Method Using Dual Spaces For The Lagrange Multiplier. *SIAM J. Numer. Anal* 38: 989-1012, 1998.

Title: Impact of Material Heterogeneity on the Fracture Properties of Asphalt Mixtures

Author(s): Jaime Wills, Silvia Caro, *U. Los Andes*; Andrew Braham, *U. Arkansas*.

Design, analysis, and construction processes in civil engineering require a detailed knowledge of the response and performance of the materials to be used in each project. Computational modeling techniques are efficient tools that can be applied to support this objective. Nevertheless, developing accurate mechanical models of materials, especially for most composite materials regularly used in pavement engineering, represents a challenge, mainly due to their intrinsic heterogeneity. In the laboratory, the role of material heterogeneity in the determination of material properties is controlled by testing a minimum number of replicates, and by defining maximum acceptable values of dispersion among these results. However, probabilistic and stochastic principles could be used in combination to more classical computational mechanical techniques to better understand the impact of material variability during these characterization processes. Within this context, this investigation begins by summarizing recent works that have been reported in the literature to model the heterogeneity of Hot Mix Asphalt (HMA) specimens in standardized experimental tests. After describing these previous efforts, this work presents a technique to assess the effect of material variability in the dispersion reported among results from multiple replicates of the same designed material through the HMA Semi Fracture bending test (SCB) (ASSHTO TP 105 - 13). This technique captures material heterogeneity by applying the stochastic method of Random Fields (RM) in order to create numerical specimens with variable mechanical properties. These numerical specimens are later used to model the SCB test in the commercial Finite Element Model (FEM) Abaqus®, using a linear viscoelastic constitutive relationship and a Cohesive Zone Modeling (CZM) approach. Thus, the modeling approach recreates material heterogeneity in a macroscopic scale, as a function of the expected microstructural variability of HMA specimens. This work sets a foundation to integrate currently available numerical modeling techniques, with the objective of evaluating the impact of HMA heterogeneity and variability in the reliability associated to the results provided by most standardized tests currently used in pavement engineering.

Title: Failure Mechanism of Aluminum via Atomistic Simulation

Author(s): Nicholas Winter, Liuyang Zhang, Xianqiao Wang, *UGA*; Matthew Becton, .

Nanoporous metals with a 3D, bicontinuous, interpenetrating, ligament-channel structure show tremendous applicability in fields such as catalysis, sensing, and energy systems. This paper presents a molecular dynamics case study that investigates the failing mechanisms of nanoporous aluminum and how porosity, ligand size, and temperature affect the mechanical properties of this material under the stresses of uniaxial tension. The nanoporous aluminum was modeled using a phase field method that defines the spinoidal separation of a binary fluid, devised by John Cahn and John Hilliard. We show that plastic failure in nanoporous aluminum begins with the emission of dislocation loops in the junctions between ligands, stacking faults then begin to accumulate in ligands in the loading direction, and these stacking faults result in the necking and breakage of ligands. We also investigate the scaling laws of young's modulus, yield strength, and ultimate strength using the relationships proposed by Gibson and Ashby.

Title: Modeling Topological Effects on Multi-Phase Fluids: Self-Lubricating, Self-Healing and Self-Cleaning Surfaces

Author(s): Olga Wodo, *U. Buffalo, SUNY*; Baskar Ganapathysubramanian, *Iowa State U.*

Hierarchical nanostructured surfaces offer the possibility of multiple functionalities with important application for self-cleaning, anti-icing or drag-reduction in micro-channels. A quintessential example is the 'lotus effect' which is the result of roughness induced superhydrophobicity, such that texturing prevents droplets from filling the pits. Another promising application is when systematically patterned holes and grooves are filled with lubricant to provide enhanced transport properties when in contact with another immiscible fluid (such as water on oil infused surfaces). Establishing structure-property relations is crucial for designing the texture of the surface to tailor the functionality. A necessary prerequisite, thus, is to understand the topological aspect of the interface between two immiscible fluids (e.g. water and oil, water and air) To study topological aspects of the multiphase systems, we develop a diffuse interface computational model for immiscible multi-phase flow. We couple the Navier-Stokes equation with Cahn-Hilliard equation to account for multi-component fluid flows and the interfacial phenomena. We detail the temporal and spatial challenges faced in numerically solving the set of equations. We address these 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. Using this approach, we study the interface stability in oil infused grooved substrates. We analyze geometrical aspect of the grooved substrate searching for optimal textures providing slip and maintaining stability of the interfaces.

Title: Application of the Method of Difference Potentials to Linear Elastic Fracture Mechanics

Author(s): Huw Woodward, Sergei Utyuzhnikov, *U. Manchester*, Patrick Massin, *UMR EDF*.

The Difference Potential Method (DPM) [1] proved to be a very efficient tool for solving boundary value problems (BVPs) in complex regions. A well-defined auxiliary problem is used to reduce BVPs to a boundary equation without the knowledge of Green's functions. The method has been successfully used for solving very different problems related to the solution of partial differential equations [1]. Recently the DPM has been applied to Linear Elastic Fracture Mechanics [2]. Singular enrichment functions, such as those used within the Extended Finite Element Method, were introduced in order to improve the approximation near to the crack tip. Near-optimal convergence rates were achieved. In [2] the problem was reduced to a grid boundary close to the physical boundary of the problem. The problem is now further reduced to a system of basis functions introduced along the physical boundary of the problem, as suggested in [1] for regular problems. The basis functions form an approximation of the trace of the solution at the physical boundary. This method has proven efficient for the solution of problems on regular (Lipschitz) domains, e.g. [3]. In the current work the boundary basis is enriched near the crack tip in order to account for the singularity. Local splines are used for the basis functions to localise any error caused by the singularity. Further to this the interpolation to the auxiliary grid nodes must also account for the singularity close to the crack tip. When higher-order, equation-based interpolations are used, such as those used by [3], competitive convergence rates are achieved for a fully enriched formulation. The method is a significant development upon [2] as the number of unknowns of the system is reduced; leading to the need for much fewer solutions of the auxiliary problem, and the application of boundary conditions of all kinds is more straightforward. [1] Ryaben'kii V.S., Method of Difference Potentials and Its Applications. Springer-Verlag, Berlin, 2002. [2] Woodward WH, Utyuzhnikov S, Massin P, On the Application of the Method of Difference Potentials to Linear Elastic Fracture Mechanics. International Journal for Numerical Methods in Engineering, 2015 (in press). [3] Medvinsky M, Tsynkov S, Turkel E. The method of difference potentials for the Helmholtz equation using compact high order schemes. Journal of Scientific Computing 2012; 53(1):150–193.

Title: Ramifications of Post Processing on Geometrically Necessary Dislocation Calculations from EBSD-Based Orientation Measurements

Author(s): Stuart I. Wright, Matthew M. Nowell, *EDAX*; David P. Field, *Washington State U.*

The use of automated Electron Backscatter Diffraction (EBSD) to map the lattice orientation in crystalline materials has become an established tool for characterizing deformed microstructures. The spatially specific crystallographic orientation information provided by this technique is critical to understanding the evolution of microstructure during deformation. Models based on such measurements rely on robust and precise orientation measurements. The precision is particularly important when investigating the small angle rotations induced by the generation of dislocations and their movement through the microstructure. While not all dislocation characteristics can be extracted from the EBSD based orientation data it is possible to quantify the density of Geometrically Necessary Dislocations (GND) from the local variations in orientation captured by EBSD. Unfortunately, these local orientation perturbations are typically right at the limit of angular precision of EBSD. Recent results on orientation precision [1] show that some improvement in orientation precision can be achieved through careful selection of indexing parameters. Cross-correlation methods can also achieve very high levels of precision, but very high quality and high resolution patterns are required for such measurements. The time needed to collect such patterns makes it intractable to characterize deformed microstructures over areas containing more than just a few grains. For conventional EBSD mapping, several post-processing tools have been developed in an effort improve the angular precision. However, these routines generally give the impression of improved orientation precision through point-to-point smoothing of the orientation data within the measurement grid. A post processing approach which improves indexing performance through noise reduction in the patterns through local averaging of patterns also tends to reduce local orientation variations. The ramification of these post processing methodologies in terms of GND calculations is explored. [1] S. I. Wright, M. M. Nowell, R. de Kloe and L. Chan (2014) "Orientation Precision of Electron Backscatter Diffraction Measurements near Grain Boundaries", *Microscopy and Microanalysis* 20, 852-863.

Title: Mesoscale Analysis of Crack-Induced Diffusivity of Concrete Through a Phase-Field Modeling Approach

Author(s): Tao Wu, Laura De Lorenzis, *Tech. U. Braunschweig*.

A variety of durability problems in cement and concrete are the result of the interaction of diffusion processes combined with chemical reactions, such as the attack of chloride ions. Cracks have large impact on increasing the diffusivity of concrete since they provide low-resistance pathways for chloride ions, such that the attack process of chloride ions is accelerated. The objective of this work is to numerically investigate the influence of cracks on the diffusivity of concrete. Concrete is a heterogeneous material which is comprised of cement paste and aggregates. In this work, the mesoscale heterogeneity of concrete is explicitly characterized by the presence of randomly distributed spheres embedded in the homogeneous cement paste. Cracking is described by a phase-field modeling approach, which is capable of handling arbitrarily complex topologies of the crack surfaces, including branching and merging, on a fixed mesh. The diffusion of chloride ions in concrete is modeled by Fick's law. The dependency of the diffusivity of concrete on the crack width, which is obtained from the experimental results, provides the basis for the diffusion-mechanical coupling. The latter is implemented using a staggered algorithmic formulation. Comparisons between numerical and experimental results are also illustrated.

Title: Analysis of Impact Penetration Using a Lagrangian Particle Formulation

Author(s): Youcai Wu, *Karagozian & Case* ; John Crawford, Hyung-Jin Choi, *Karagozian & Case*.

Abstract A Lagrangian particle formulation is developed and applied in the analysis of high strain rate impact failure processes. The formulation couples the finite element (FE) and reproducing kernel (RK) formulation [1, 2] on the fly and changes from the more computationally efficient FE formulation to the more computationally robust RK formulation when certain triggering criteria are satisfied. State variables such as material damage or effective plastic strain are employed as the triggering criteria so that the RK approximation is only applied in the highly distorted regions (i.e., ones exhibiting high damage or effective plastic strain). By doing so, such a coupled formulation takes advantage of the benefits afforded by both the FE and RK formulations while minimizes the disadvantages of each. The weak form of the coupled approximation is integrated uniquely by a stabilized conforming nodal integration technique [3, 4] so that no state variable transition is needed when the approximation is converted from FE to RK. This not only guarantees the efficiency of the formulation, but also, more importantly, maintains the accuracy during the conversion, and avoids special treatments such as the interpolation that may be needed to transfer the variables from different sets of material points (i.e., the Gauss points in Gauss quadrature) of standard FE formulation and the nodal points of a particle formulation. The nodal integration also preserves the particulate nature of the particle method so that the formulation is suitable for analyzing high strain rate impact failure processes where large degree of material damage and separation occurred, which are very difficult for finite element method (sometimes no solution can be obtained at all). This formulation also allows a natural way to capture debris evolution, which is of great interest in many impact penetration analyses. Several examples including impact failure of concrete and steel materials are analyzed using the Lagrangian form of coupled FE/RK approximation are presented which demonstrates very good correlation with experimental observations. Reference: 1. Wu Y., Wang D., and Wu C.T. "A direct displacement smoothing meshfree particle formulation for impact failure modeling," International Journal of Impact Engineering, submitted, 2015 2. Wu Y., Magallanes J.M., and Crawford J.E. "Fragmentation and debris evolution modeled by a point-wise coupled reproducing kernel-finite element formulation," International Journal of Damage Mechanics, 23, 1005-1034, 2014 3. Chen J.S., Wu C.T., Yoon S., You Y. "A stabilized conforming nodal integration for Galerkin meshfree methods," International Journal for Numerical Methods in Engineering; 50, 435-466, 2001 4. Chen J.S., Yoon S., Wu C.T. "Nonlinear version of stabilized conforming nodal integration for Galerkin meshfree methods," International Journal for Numerical Methods in Engineering; 53, 2587-2615, 2002

Title: Advanced FSI Simulation of Wind Turbine Rotor–Tower Interaction

Author(s): Michael C. H. Wu, Carolyn N. Darling, Chenglong Wang, Ming-Chen Hsu, *Iowa State U.*;
Dominik Schillinger, *U. Minnesota*.

In this work, fluid–structure interaction (FSI) technique is employed to study a full wind turbine machine, including rotor–tower aerodynamic interaction, and rotor–tower structural interaction. The aerodynamic interaction was simulated and validated in Hsu et al. [1, 2]. To study the structural interaction, it is critical to model a shaft connecting the nacelle and the hub, to properly couple the interaction between a rotating rotor and deformable tower. Instead of meshing the actual shaft that connects the hub and nacelle geometries, we developed a penalty-based formulation to model such function. The FSI simulation proposed in the work will provide valuable information of the coupled interaction among the air flow, rotating rotor, and deformable structures such as blades, nacelle and tower. REFERENCES [1] Hsu M-C, Akkerman I, Bazilevs Y (2014) Finite element simulation of wind turbine aerodynamics: Validation study using NREL Phase VI experiment. *Wind Energy* 17:461-481. [2] Hsu M-C, Bazilevs Y (2012) Fluid–structure interaction modeling of wind turbines: simulating the full machine. *Computational Mechanics* 50:821-833.

Title: A Displacement Smoothing Induced Strain Gradient Stabilization for the Linear and Non-Linear Meshfree Galerkin Nodal Integration Method

Author(s): C.T. Wu, *LSTC*.

Inspired by the Galerkin/least-squares (GLS) stabilization approach developed by Beissel and Belytschko [1], we introduce a gradient-type stabilization formulation to the meshfree Galerkin nodal integration method for linear and nonlinear solid mechanics analyses. The stabilization is introduced to the standard variational formulation through an enhanced strain induced by a decomposed smoothed displacement field [2] using the first-order meshfree convex approximations [3]. It leads to a penalization formulation containing a symmetric strain gradient stabilization term for the enhancement of coercivity in the direct nodal integration method. As a result, the stabilization parameter comes naturally from the enhanced strain field and provides the simplest means for effecting stabilization. The numerical results of the present method in linear analysis indicate that the stress-error norm and the norm of penalty error are close to an optimal convergence rate of $O(h)$. Both quasi-static and explicit dynamic analyses are considered in the nonlinear applications. Several numerical benchmarks are examined to demonstrate the effectiveness and accuracy of the proposed stabilization method for the nodal integration simulation of large deformation problems. Reference 1. Beissel S, Belytschko T (1996) Nodal integration of the element-free Galerkin method. *Comput Methods Appl Mech Eng* 139:49-74. 2. Wu CT, Guo Y, Hu W (2014) An introduction to the LS-DYNA smoothed particle Galerkin method for severe deformation and failure analysis in solids. 13th International LS-DYNA Users Conference, Detroit, MI, June 8-10, pp1-20. 3. Wu CT, Park CK, Chen JS (2011) A generalized approximation for the meshfree analysis of solids. *Int J Numer Methods Engrg* 85:693-722.

Title: Element-Size Gradation in an Unstructured Tetrahedral Mesh Using Radial Basis Functions

Author(s): Nick Wyman, Mike Jefferies, Steve Karman, John Steinbrenner, *Pointwise, Inc.*.

Generation of a constrained tetrahedral mesh with a prescribed element size gradation requires knowledge of the desired element size at discrete locations in the domain. User control of element size gradation is provided through the constraining surface mesh, optional primitive (curve and surface) shape sources, influence parameters, and a background mesh size. These user controls, while convenient and natural, are in a form difficult to translate to an arbitrary point in the domain. Furthermore, if the input is inconsistent, which is common in the authors' experience, discontinuities in the desired element size field can be created leading to poor mesh quality. We propose a method for general interpolation of a user prescribed element size field which also minimizes the effect of inconsistent input. A method for defining and interpolating a target 3D element size field utilizing radial basis functions (RBF) will be described. The process begins with the conversion of the constraining surface mesh and optional primitive shape sources into an equivalent element size field represented by radial basis functions. In our method, each RBF provides local target element size using a linear distance function. Selection of a linear distance function for element size allows for natural definition of the input influence parameter also known as the element growth rate. Furthermore, an individual RBF is only effective within a distance defined by the background mesh size and the influence parameter. Each constraining surface point contributes an RBF formed from the local surface element size, the influence parameter, and the background mesh size. Our application utilizes non-uniform rational basis spline (NURBS) curves and surfaces for primitive shape definition. Target element size and influence parameters are assigned at parametric locations within the NURBS definition. A discrete tessellation of the NURBS shape is then created with each point generating an RBF. Finally, the desired element size at a discrete position is calculated from a blend of the effective RBFs in the region. Results from a variety of weighting schemes will be presented along with efficiency gains introduced through the use of oct-tree sorting of the RBFs.

Title: Experiment and Numerical Simulation of Concrete Structure Damage Under Impact Loading

Author(s): Xu Xiangzhao, Ning Jianguo, *Beijing Inst. Tech.*; Wang Zhihua, *Taiyuan U. Tech.*.

Concrete material has extremely complex dynamic characteristics which used in structural engineering with a history of nearly hundred years and has important application in the field of national defense [1]. The concrete structure used in protection works has higher reinforcement ratio and thicker thickness than in engineering [2]. It is extremely difficult to destroy such high reinforcement ratio and thick concrete walls effectively. A software platform which can study on numerical simulation of impact problem was developed based on the Euler method [3]. The numerical simulation of shaped charge with different type cone angle liners were studied by independent development software, and the forming rules of shaped charge with different type cone angle liners were obtained. A shaped charge structure which can penetrate the thick concrete target was designed according to the performance parameter of penetrator by numerical simulation. The different blasting height of shaped charge penetrating concrete target was simulated and the best blasting height was obtained. The experiment of the designed shaped charge structure was tested and the test results show that concrete target size has a significant effect on penetration. The target damage is difficult to estimate because this problem was belonging to discontinuity, while the software is developed based on the continuity assumption, which makes the numerical simulation of target damage very difficult. In order to solve this problem the damage identification was added in post-processing software, the overall damage of the target can be approximately obtained by observing the different time numerical simulation images of destruction. This method was adopted to estimate the size of concrete target and the destruction. The numerical results of shaped charge penetration different concrete target size were analyzed to obtain the minimum concrete target size on the premise of the test requirements. The experiment of shaped charge penetration the minimal minimum concrete target was tested. The test results verify the feasibility of software. According to the experiment and numerical simulation analysis results, the reasonable structure of shaped charge can be achieved for thick concrete penetration and the software can simulate impact problems well. [1] Forrestal M.J., Frew D.J., Hickerson J.P., Rohwer T.A.. Penetration of concrete targets with deceleration-time measurements, *Int J Impact Engng*, 2003, 28(5): 479-497. [2] Wang C., Ma T.B, Ning J.G., Experimental investigation of penetration performance of shaped charge into concrete targets, *Acta Mechanica Sinica*, 2008, 24(3): 345-349 [3] Ma, T.B., Wang, C., Ning, J.G., Numerical study on the shaped charges, *International Journal of Modern Physics B*, 2008, 22(31-32): 5749-5754.

Title: Ensemble-Based Inverse Modeling and Its Application in Uncertainty Quantification of Turbulent Flow Simulations

Author(s): Jian-Xun Wang, Heng Xiao, *Virginia Tech.*

Computational Fluid Dynamics simulations, particularly those based on Reynolds Averaged Navier-Stokes (RANS) solvers, are widely used in the analysis, design, and optimization of engineering devices and structures such as pumps, turbines, and propellers. Significant uncertainties are present in these simulations, which can be mainly attributed to two sources: (1) input uncertainties due to the characterization of operation conditions and the limited manufacturing precisions, and (2) model-form uncertainties (MFU) due to the modeling errors of the Reynolds stresses in the RANS equations. The two sources of uncertainties and their interactions pose great challenges to the effective use of CFD in engineering practices [1]. Quantification and reduction of these uncertainties are crucial for proper interpretation of the CFD simulation results and for the decision-making processes based thereon. In this work, we take advantage of a physics-based parameterization strategy for Reynolds stress modeling errors, and utilizes an ensemble-based inverse modeling method to quantify and reduce the model-form uncertainties associated with the Reynolds stresses. By combining the physical prior knowledge of the flow and the properties of the turbulence model of concern with available observation data (either from experiments or from higher fidelity simulations such as Large Eddy Simulations), the proposed strategy is able to quantify and reduce the model-form uncertainty. Consequently, the input uncertainties are faithfully propagated to the uncertainty distribution in the quantity of interest. Compared to traditional methods of MFU quantification based on simple, stationary Gaussian processes [2], where computational solvers are treated as black boxes, the current methodology represents a more efficient usage of the data (which are often sparse and difficult to obtain) and the physical knowledge. The proposed method is applied to several canonical flow problems of engineering relevance, and its merits are preliminarily illustrated. [1] J.-X. Wang, C. J. Roy and H. Xiao. A Multi-Model Approach for Uncertainty Propagation and Model Calibration in CFD Applications. Arxiv Preprint, arxiv:1501.03189 [2] M. C. Kennedy, A. O'Hagan, Predicting the output from a complex computer code when fast approximations are available, *Biometrika* 87 (1) (2000) 1–13.

Title: Analysis of Interacting Surface Cracks Using the S-Version Finite Element Method

Author(s): Wei Xie, *Northwestern Polytech. U.*

Failure due to multiple cracks is one of the most common problems in ageing aircraft, pressure vessel and piping components. How to quantitatively estimate the interaction of multiple cracks is currently one of the important topics in the field of fracture mechanics. It is well known that the finite element method (FEM) is the most general method. However, FEM requires a special mesh mapping around the crack tip. FEM is generally extremely time consuming, and its accuracy is not high if numerous cracks are studied. For this reason many new techniques that can carry out crack analysis without rebuilding the finite element model have been proposed, such as X-FEM [1] and s-FEM [2]. In this talk, the formulation of s-FEM incorporated with multiple crack problems is presented first and then the implementation of VCCM [3] in s-FEM technique is discussed. The technique was applied for the issues of two dissimilar coplanar or non-coplanar surface cracks in a plate subjected to remote tension. The meshes localized to crack fronts are built individually and superimposed onto the global mesh of the overall structure. The stress intensity factors along the crack fronts were then computed, and the interaction factors of the two cracks were estimated. The influences of the crack shape parameter and the relative crack location on the interaction factors are considered. The solutions presented can be used to assess fail-safe conditions and fatigue crack growth for the situation with multiple three-dimensional cracks. Acknowledgement The authors would like to thank the financial support by National Natural Science Foundation of China (No.11102158), the Natural Science Basic Research in Shaanxi Province of China (No. 2013JQ1004), and the 111 Project (B07050). Wei Xie would like to thank Prof. Masanori Kikuchi for assistance with the s-FEM. Reference [1] Chopp DL, Sukumar N. Fatigue crack propagation of multiple coplanar cracks with the coupled extended finite element/fast marching method. *International Journal of Engineering Science*, 2003, 41(8):845–869 [2] Masayuki Kamaya, Eiichi Miyokawa, Masanori Kikuchi. Growth prediction of two interacting surface cracks of dissimilar sizes. *Engineering Fracture Mechanics*, 2010, 77:3120-3131 [3] Hiroshi Okada, Mayumi Higashi, Masanori Kikuchi, etc. Three dimensional virtual crack closure-integral method (VCCM) with skewed and non-symmetric mesh arrangement at the crack front. *Engineering Fracture Mechanics*, 2005, 72:1717-1737

Title: ICME Research of Additive Manufacturing: Case Study of Ti-6Al-4V

Author(s): Wei Xiong, Fuyao Yan, Greg Olson, *Northwestern U.*

Due to complex thermal history in as-built alloys by additive manufacturing, property control by designing microstructure in materials is a grand challenge for both experiments and simulation. In this work, the microstructural evolution of Ti64 alloys is studied systematically in order to optimize processing parameters. ICME (Integrated Computational Materials Engineering) tools are applied for analyzing and designing laser melting process, post-heat treatment (including HIP-Hot Isostatic Pressing) of as-built alloys. Diffusion simulation was performed using the Thermo-Calc and DICTRA software in order to study the homogenization process in HIP and phase transformations during heat treatment. This work demonstrates the application of the integrated method of simulation and experimental techniques for additive manufacturing. The successful materials design of the additive manufactured alloys requires more study on microstructure control as well as CALPHAD (CALculation of PHase Diagrams) database development.

Title: Local Polynomial Chaos Method for Large-Scale Stochastic Problems

Author(s): Xueyu Zhu, Dongbin Xiu, *U. Utah*; Yi Chen, *Purdue U.*

We present a localized polynomial chaos expansion for PDE with random inputs. Our focus is on linear stochastic problems with high dimensional random inputs, where the traditional polynomial chaos methods, and most of the existing methods, incur prohibitively high simulation cost. The local polynomial chaos method employs a domain decomposition technique to approximate the stochastic solution locally. In each subdomain, a subdomain problem is solved independently and, more importantly, in a much lower dimensional random space. In a post-processing stage, accurate solution samples of the original stochastic problems are obtained by enforcing the correct stochastic structure of the random inputs and the coupling conditions at the interfaces of the subdomains. Overall, the method is able to solve stochastic PDEs in very large dimensions by solving a collection of low dimensional local problems and can be highly efficient. We present the general mathematical framework of the methodology and use numerical examples to demonstrate the properties of the method.

Title: A Variational Multi-Scale Framework for Buoyancy Driven Natural Convection

Author(s): Songzhe Xu, Chenglong Wang, Ming-Chen Hsu, Baskar Ganapathysubramanian, *Iowa State U.*

We present a coupled Variational Multiscale formulation for the turbulent buoyancy driven natural convection problem. In this framework the Navier-Stokes equation and energy equation are solved separately using a block iteration approach. We explore how various levels of approximation of the Jacobian results in increasing accurate and fast convergence and compare with the computational complexity involved. The framework is validated by the benchmark Rayleigh Benard problem for Rayleigh numbers from 10^3 up to 10^{10} , illustrating the capability of the framework to seamlessly capture laminar, transient and turbulent natural convection. We finally illustrate architectural application of the framework by exploring the effects of various architectural configurations of a building (the Interlock House) on its thermal and flow dynamics.

Title: Immersogeometric Analysis of Turbulent Flow Over Complex Geometries

Author(s): Fei Xu, Chenglong Wang, Sean Wasion, Bryann Sotomayor-Rinaldi, Ming-Chen Hsu, *Iowa State U.*; Vasco Varduhn, Dominik Schillinger, *U. Minnesota*; David Kamensky, *UT Austin*.

In this work we develop an immersogeometric framework based on tetrahedral finite elements for the simulation of flow over objects with complex geometries. The object is immersed into a locally refined, non-boundary-fitted fluid mesh to avoid the challenges associated with boundary-fitted mesh generation. A workflow based on an open-source mesh generator with parametric input is developed that fully automates the generation of adaptive non-boundary-fitted meshes. To resolve the geometry in intersected elements, an adaptive quadrature rule based on the recursive split of elements is implemented. Dirichlet boundary conditions in intersected elements are enforced weakly in the sense of Nitsche's method. The framework is implemented in an existing finite element fluid code based on the variational multi-scale method. To assess the accuracy of the proposed method, we perform computations of the benchmark problem of flow over a sphere for a wide range of Reynolds numbers, including turbulent flow up to $Re = 3,700$. Quantities of interest such as drag coefficient, Strouhal number and the pressure distribution over the sphere are in good agreement with corresponding results obtained with standard boundary-fitted approaches. Particular emphasis is placed on studying the importance of the geometry resolution in intersected elements. The results show that a faithful representation of the geometry is crucial for accurate high-fidelity flow analysis. Finally, we demonstrate the effectiveness of the immersogeometric framework in engineering applications, for example the aerodynamic analysis of tractor-trailer for drag reduction and the airflow within buildings for comfort assessment.

Title: Assessment of the Feasibility for Using Statistical Shape Analysis for Material Characterization of the Human Right Ventricle

Author(s): Jing Xu, John Brigham, *U. Pittsburgh.*

Pulmonary hypertension (PH) is a severe cardiopulmonary disease resulting in dysfunction and failure of the right ventricle (RV). Yet, there is limited capability to judge both the early stages of this deadly disease, as well as the likelihood of progression to heart failure. A core hypothesis driving the present research program is that the size, shape, and material properties of the right ventricle are intimately linked to the state of PH and would be critical guides to judge disease progression and the need for intervention. Thus far, this research group has developed and investigated statistical shape analysis approaches to identify fundamental shape and kinematic features encoded within the RV surface that could be potentially related to PH pathology [1]. The present study seeks to investigate the ability to use these same shape analysis methods to form a strategy for nondestructive and noninvasive (i.e., clinically applicable) inverse material characterization of the human RV wall. As such, a numerical study will be presented to show the potential for forming inverse characterization objectives from shape analysis results of the RV. First the computational procedure for statistical shape analysis will be presented. In particular, this shape analysis includes an anatomically consistent approach to topologically map any RV closed surface to a consistently quantitatively comparable reference surface. Then, a numerical sensitivity study will be used to display the material characterization capability. A test model of the human RV is utilized, which was derived from an arbitrary non-hypertensive human subject's MRI dataset. A finite element model was created for the RV and the pressure waveforms were applied as boundary conditions to provide a simplified simulation of the RV motion during diastole. The sensitivity of the shape analysis results will be presented with respect to both global and local (i.e., heterogeneous) changes in the heart wall material properties. Lastly, a simulated inverse problem will be presented to evaluate the potential characterization capability in which a standard optimization-based inverse solution estimation procedure is applied with objective functions derived from the shape analysis results for a set of simulated material property scenarios. [1] J. Wu, Y. Wang, M.A. Simon, and J.C. Brigham (2012), "A New Approach to Kinematic Feature Extraction from the Human Right Ventricle for Classification of Hypertension: a Feasibility Study," *Physics in Medicine and Biology*, 57, 23, December, 7905-7922.

Title: Computational Modelling of Fluid-Driven Fracture in 3D

Author(s): Guoquiang Xue, Lukasz Kaczmarczyk, Chris Pearce, *U. Glasgow.*

Hydraulic fracture (fracking), as an important technique, is widely used in Engineering. The modeling of fracking is the typical fluid-driven fracture processing by which a fracture initiates and propagates due to hydraulic loading (i.e., pressure) applied by a fluid inside the fracture. Therefore, herein mainly focuses on how the hydraulic loading works in the crack and makes the crack propagate. In this work, the rock deformation is assumed to be elastic and the leak-off is not considered at this stage. The 3D computational model is being built using the finite element method (FEM) and utilizes a hierarchic approximation basis [1], allowing for local p-refinement. The effect of the hydraulic loading is analyzed from two aspects: static and dynamic. In the static state, the problem of fracking is considered to be the 'static or quasi-static' situation. That is to say, the fluid flow is considered to be constant along the fracture but the distribution of pressure is related to the cohesive zone. Propagating fractures are modeled using zero-thickness cohesive interface elements, which has been adopted by most of fracking models and its performance will be studied. In addition, the local arc-length control methodology is used to control and analyze dissipative load path [2]. On the other hand, the dynamic hydraulic loading is researched and modeled by the potential flow model, which describes the fluid movement in a rock fracture. All problems are undertaken in 3D and the model performance will be demonstrated on a number of benchmark problems, illustrating the propagation of fluid-driven fractures. The model is being incorporated into our open source software package MoFEM [3] and is optimized for high performance computing on distributed memory computers. Key Words: fluid-driven fracture; hierarchic element; cohesive interface element; local arc-length control; potential flow; MoFEM References: [1] M. Ainsworth, J. Coyle, Hierarchic finite element bases on unstructured tetrahedral meshes, *International Journal for Numerical Methods in Engineering* 58 (14) (2003) 2103–2130. [2] G. Alfano, M. A. Crisfield, Solution strategies for the delamination analysis based on a combination of local-control arclength and line searches, *International Journal for Numerical Methods in Engineering* 58 (7) (2003) 999–1048. [3] L. Kaczmarczyk (Manager), Mesh Orientated Finite Element Method - (MoFEM v0.0.1), Department of Civil Engineering, School of Engineering, The University of Glasgow, Glasgow, G12 8LT, available at: <https://bitbucket.org/likask/mofemjoseph> (2015).

Title: Uncertainty Quantification of High-Dimensional Complex Systems by Hybrid Polynomial Dimensional Decomposition Method

Author(s): Vaibhav Yadav, *San Diego State U.*; Sharif Rahman, *U. Iowa.*

This paper presents a novel hybrid polynomial dimensional decomposition (PDD) method for stochastic computing in high-dimensional complex systems [1]. When a stochastic response does not possess a strongly additive or a strongly multiplicative structure alone, then the existing additive and multiplicative PDD methods [2, 3] may not provide a sufficiently accurate probabilistic solution of such a system. To circumvent this problem, a new hybrid PDD method is developed that is based on a linear combination of an additive and a multiplicative PDD approximation, a broad range of orthonormal polynomial bases for Fourier-polynomial expansions of ANOVA component functions, and a dimension-reduction or sampling technique for estimating the expansion coefficients. A theorem and a corollary are proven giving the analytical expressions for the model parameters that form the linear combinations of additive PDD and multiplicative PDD approximations, resulting in the hybrid PDD method. Explicit formulae are also derived for calculating the response moments by the univariate hybrid PDD approximation. The univariate truncation of hybrid PDD is employed to calculate the probabilistic characteristics of simple dynamic systems subjected to random input parameters. The univariate hybrid PDD approximation is found to be more accurate than either the univariate additive or multiplicative PDD methods, and is more efficient than the bivariate additive PDD method in determining the tail probabilistic characteristics of the random. Finally, a successful evaluation of random eigensolutions of a pickup truck, subjected to 46 input random variables, involving coupled acoustic-structure analysis demonstrates the ability of the new method in solving large-scale practical engineering problems. References: [1] Yadav, Vaibhav, and Sharif Rahman. A hybrid polynomial dimensional decomposition for uncertainty quantification of high-dimensional complex systems. *Probabilistic Engineering Mechanics* 38 (2014): 22-34. [2] Yadav, Vaibhav, and Sharif Rahman. Uncertainty quantification of high-dimensional complex systems by multiplicative polynomial dimensional decompositions. *International Journal for Numerical Methods in Engineering* 94, No. 3 (2013): 221-247. [3] Rahman, Sharif. A polynomial dimensional decomposition for stochastic computing. *International Journal for Numerical Methods in Engineering* 76, no. 13 (2008): 2091-2116.

Title: Wavelet Transformation Induced Multi-Time Scaling (WATMUS) Model for Coupled Transient Electro-Magnetic and Structural Dynamics Finite Element Analysis

Author(s): Reza Yaghmaie, *Johns Hopkins U.*; Somnath Ghosh, *Johns Hopkins U.* .

This paper proposes a multi-temporal computational model for modeling functional materials with electro-magneto-mechanical couplings which appear in stretchable antennas for wireless power harvesting and communications, piezoelectric sensors, actuators and MEMS. The proposed method serves as a unified guide to the numerical implementation of the time dependent coupled electro-magneto-mechanical problems on a macroscopic temporal level. Macro-micro temporal constitutive statements based on global variational principles, which govern the representing evolutions of internal variables are developed. Consequently, incremental boundary value problems representing transient electromagnetic effects under dynamic mechanical loadings and associated finite element discretization appear in the form of global variational statements. The Euler-Lagrange equations of the corresponding (Hamilton's) variational principle are Gauss' and Ampere's equations that are solved using Newton-Krylov Method. Characteristics of the coupled solutions clearly demonstrate the complexity brought about by coupling the two physical phenomena. The fields governing the response naturally have large discrepancies in the frequencies viz. the ultrasonic electromagnetic field frequencies and the low mechanical vibration frequencies and this involves simulating a large number of electromagnetic cycles. A conventional single time-scale analysis proceeds in the time-scale of the highest frequency response and hence it is challenging to address issues related to the low frequency field. The present work addresses these issues by introducing a novel wavelet transformation based multi-time scaling method (WATMUS) for coupled transient electromagnetic nonlinear dynamical mechanical simulations in the finite element framework. This method is advantageous over conventional methods that fail because of assumptions of periodicity etc., because no assumption of scale separation is needed with this method. The WATMUS method also provides an implicit framework to perform coarse scale integration and hence does not exhibit stability issues. The wavelet transformation projects the high frequency (fine time scale) transient electromagnetic potential response through translation and dilation of an appropriate set of scaling functions on the low frequency (coarse time scale) mechanical response with monotonic evolution. The multiresolution based discrete wavelet families are used for accurate representation of any complex electromagnetic responses. The method significantly enhances the computational efficiency in comparison with conventional single time scale integration methods. The WATMUS scheme is also improved by an adaptive method to determine the optimal coarse time scale step sizes and construct the number of evolving wavelet coefficients. The method is used to solve a real application antenna dish structure problem to prove the accuracy and computational efficiency of the WATMUS method in comparison with single time scale methods. The proposed WATMUS methodology is found to have a tremendous potential in accurately simulating large number of electromagnetic cycles arising in real application multi-physics problems.

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Title: Balancing Domain Decomposition Method with Additive Schwartz Framework for Complex Structures

Author(s): Tomonori Yamada, Shinobu Yoshimura, *U. Tokyo.*

An iterative substructuring method with coarse grid correction, such as balancing domain decomposition(BDD) method, is one of the most effective approaches for parallel computing of large scale structural finite element analyses. In the balancing domain decomposition by constraints(BDDC), the coarse problem is applied in an additive manner, while in BDD, it is applied multiplicatively. Here, computing performance of the BDD method with additive Schwartz framework for complex structures is investigated in this research.

Title: Error Estimation Based on Method of Nearby Problems for Finite Element Analysis of Nonlinear Solid Mechanics

Author(s): Takahiro Yamada, *Yokohama Nat'l. U.*

The method of nearby problems developed by Roy et al. is a sophisticated error estimation and solution verification procedure, in which the problems with exact solutions near the target problem of interest can be generated by a curve fitting of a numerical solution to a continuous function. In this work, we propose a formulation and procedure to apply the method of nearby problems to the nonlinear finite element analysis of solid. In our approach, the solution of nearby problems is constructed by the projection of a finite element solution of displacement onto function space of spline using the inner product in the Sobolev space H^1 . The spline is a polynomial function that possesses a sufficiently high degree of smoothness. The Sobolev space H^1 is a suitable function space to deal with the second order partial differential equations such as governing equations in solid mechanics. The combination of spline function and projection using the H^1 inner product gives the suitably smooth function fitted to the given numerical solutions owing to the product of the first derivatives of the functions in the inner product. In this work, the uniform tensor product B-spline functions are employed and complex geometry is considered by using the fictitious domain approach. To calculate the body force (source term), the weak formulation is adopted in order to avoid calculation of the second order derivative of the solution of nearby problems. Then the actual procedure to calculate equivalent nodal force derived from the given solution is similar to evaluation of internal force, in which the work product of the stress and virtual strain is integrated over the domain. We can apply our procedure to the problem, including material nonlinearity such as elasto-plasticity. Therefore, we obtain a numerical procedure for error estimation and solution verification for solid problems including elasto-plasticity that is hardly found in the literatures. Several representative numerical results are also presented.

Title: Hybrid Grid and Particle-Based CFD Method for Multi-Physics Engineering Problems

Author(s): Makoto Yamamoto, *Tokyo U. Science*.

Computational Fluid Dynamics (CFD) has been completely matured in the engineering sense. Nowadays, we can use CFD for research and development of various machines. However, most targets of current CFD are limited to single-phase flows. Thus, in near future, we have to focus on multi-phase flows which are typically of multi-scale and multi-physics. Based on this consideration, I have been tackling the modeling and simulations of multi-physics engineering problems such as ice accretion, particle deposition and sand erosion in a jet engine. In these problems, the flow fields strongly depend on surface deformation. For example, ice layer whose thickness is few mm is formed on fan blades of a jet engine in icing environments. Such a thin ice layer can lead to 10% performance degradation. Therefore, exact reproduction of surface deformation is critical in the simulations. At first, I adopted a finite difference method (i.e. grid-based method) because of my long experience. Using a finite difference method, I and my students succeeded in simulating the temporal changes of flow field, wall surface and machine performance due to icing, deposition and erosion. However, in the simulations, we had to smooth the wall surface so that we could re-generate the grid along the deformed or rough surface. This might reduce or destroy the accuracy of simulations. (It is too difficult to verify and validate this point.) So, I decided to change the strategy, and introduced a particle-based method, since it does not need any grid system. It should be noted that a particle-based method has one big disadvantage, that is, it is too time-consuming. Therefore, a hybrid grid and particle-based method is recently developed. The macroscopic field is computed by a grid-based method, while microscopic or mesoscopic phenomenon on and over a wall surface is computed by a particle-based method. Doing so, I expect that this hybrid method can improve the accuracy of multi-physics simulations in both quality and quantity. In the final paper and my presentation, the numerical procedures of the hybrid grid and particle-based method is introduced, with showing the numerical results on ice accretion and particle deposition phenomena in a jet engine.

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Title: Computational Free-Surface Fluid-Structure Interaction: Aquatic Sports, Offshore Floating Wind Turbines and Numerical Wave Generation

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

Two-phase Navier-Stokes models are becoming increasingly popular for modeling free-surface flows and hydrodynamic processes. They hold particular appeal for problems where full vertical resolution is required in velocity and pressure, (e.g., short-wave phenomena, flow around coastal structures and levees, and extreme erosion processes). In this work, we propose a FSI framework using finite element and isogeometric methods, which enables the simulation of the interaction between free-surface flow and structures with great efficiency, accuracy and robustness. The formulation will be described in details and a wide range of engineering applications including tandem compliant hydrofoils for Kayak propulsion, offshore floating wind turbines and numerical wave generation will be presented.

Title: A New Heat Source Model for Electron Beam and Substrate Interaction

Author(s): Wentao Yan, *Northwestern U.; Tsinghua U.*; Jacob Smith, Wing Liu, *Northwestern U.*; Wenjun Ge, Feng Lin, *Tsinghua U.*

An electron beam is a widely applied processing tool in welding and additive manufacturing applications. The heat source model of the electron beam acts as the basis of thermal simulations and predictions of the micro-structures and mechanical properties of the final products. While traditional volumetric and surface heat flux models were developed previously based on the observed shape of the molten pool produced by the beam, a new heat source model with a physically informed foundation has been established in this work. The new model was developed based on Monte Carlo simulations performed to obtain the distribution of absorbed energy through electron-atom collisions for an electron beam with a kinetic energy of 60KeV hitting a Ti-6Al-4V substrate. Thermal simulations of a moving electron beam heating a solid baseboard were conducted to compare the differences between the new heat source model, the traditional surface flux model and volumetric flux model. Although the molten pool shapes with the three selected models were found to be similar, the predicted peak temperatures were noticeably different, which influences the evaporation, recoil pressure and molten pool dynamics. The new heat source model was also used to investigate the influence of a static electron beam on a substrate. This investigation indicated that the new heat source model could scientifically explain phenomena that the surface and volumetric models cannot, such as eruption and explosion during electron beam processing.

Title: Flow Simulations Over Array of Cylinders and Moving Cylinders via Semiclassical Lattice Boltzmann Method

Author(s): Joe Jaw-Yen Yang, Chia-Ju Wei, Wun-Yi Huang, *Nat'l. Taiwan U.*

A lattice Boltzmann method for the semiclassical Boltzmann–Ellipsoidal Statistical method equation [1] is presented. The method is derived by projecting the kinetic governing equation directly onto the tensor Hermite polynomials basis and various hydrodynamic approximations can be achieved depending on the expansion orders [2]. It is an extension of a previous semiclassical lattice Boltzmann-BGK method [3]. In the new ES model, a generalization of the classical ES model [4], besides the usual normal variables, additional higher order pressure tensor moments are needed and a corresponding decoding procedure is required. A direct solver was given in [5]. A LBM for the classical Boltzmann-ES model was presented [6]. The fluid-solid interaction is treated by immersed boundary velocity correction method and several other boundary methods. The semiclassical lattice Boltzmann-ES-BGK method can give correct and adjustable Prandtl number through a model parameter. The semiclassical hydrodynamic equations approximated by the LBM have been analyzed by the Chapman-Enskog expansion. Simulations of the hydrodynamic flows over array of cylinders and moving cylinders based on D2Q9 lattice model are illustrated for three statistics. Effects of different values of the model parameter of the ES model are to be examined and studied. [1] Wu L., Meng J. P. and Zhang Y. H., *Proc. R. Soc. A* **468**, 1799-1823, 2012. [2] Shan, X., Yuan X.F., and Chen H., *J. Fluid Mech.* **550**, 413, 2006. [3] Yang, J.Y. and Hung, L.H., *Phys. Rev. E* **79**, 056708, 2009. Coelho, R.C. et al., *Phys. Rev. E* **89**, 043302, 2014. [4] Holway, L. H., *Phys. Fluids* **21**, 593-610, 1966. [5] Yang, J.Y., et al, *Proc. R. Soc. A* **470**, 20140061, 2014. [6] Meng, J. et al, *J. Fluid Mech.*, **718** 347-370, 2013.

Title: Shock-Capturing with AMR and Artificial Viscosity on Moving Grid

Author(s): Jingjing Yang, Chunlei Liang, *George Washington U.*

An efficient AMR data structure is proposed to be integrated into a high-order solver (CPR). With artificial viscosity facilitates capturing the shock, the AMR scheme will be able to dynamically response the locations that a sensor points to and refine the grid, either fixed or moving, adaptively. By refining the grids where shock transverses or occurs, the dissipation can be reduced and a sharp profile of shock can be presented. It maximally retains the rigidness of the CPR solver. Comparing to tree-based AMR, it can be naturally extended to parallelization, and saves CPU time by avoiding recursive search in a list or tree.

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Title: A Projected Preconditioned Conjugate Gradient Method for Solving Large-Scale Eigenvalue Problems in Materials Simulation

Author(s): Chao Yang, Eugene Vencharynski, John Pask, *Lawrence Berkeley Nat'l. Lab.*

We present an iterative algorithm for computing an invariant subspace associated with the algebraically smallest eigenvalues of a large sparse or structured Hermitian matrix A . We are interested in the case in which the dimension of the invariant subspace is large (e.g., over several hundreds or thousands) even though it may still be small relative to the dimension of A . These problems arise from, for example, density functional theory (DFT) based electronic structure calculations for complex materials. The key feature of our algorithm is that it performs fewer Rayleigh--Ritz calculations compared to existing algorithms such as the locally optimal block preconditioned conjugate gradient or the Davidson algorithm. It is a block algorithm, hence can take advantage of efficient BLAS3 operations and be implemented with multiple levels of concurrency. We discuss a number of practical issues that must be addressed in order to implement the algorithm efficiently on a high performance computer.

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Title: Direct Time-Integration Method for Solving Nonlinear Dynamic Problems with Large Rotations and Displacements

Author(s): Y. B. Yang, *Nat'l. Taiwan U.; Chongqing U.*; S. R. Kuo, *Nat'l. Taiwan Ocean U.*; J. D. Yau, *Tamkang U.*

An efficient time-integration algorithm for nonlinear dynamic analysis of structures is presented. By adopting the temporal discretization for time finite element approximation, very large time steps can be used by the algorithm. With an accuracy of fourth order, this technique requires only displacements and velocities to be made available at the start of the current time step for integration in state space. Using the weighted momentum principle, the problem of discontinuity caused by impulsive loads is resolved after time-integration of the applied load in external momentum. Since no knowledge is required of acceleration at the current time step, the errors caused by estimation of acceleration by previous finite-difference methods are circumvented. Moreover, an iterative procedure is included for each time step, involving the three phases of predictor, corrector, and error-checking. The effectiveness and robustness of the proposed algorithm in solving nonlinear dynamic problems is demonstrated in the numerical examples.

Title: Nonlinear Iterative Analysis Using Reproducing Kernel Collocation Method

Author(s): Judy Yang, *Nat'l. Chiao Tung U.*

This study is concerned with the nonlinear iterative solution of problems with semilinear elliptic partial differential equations using the reproducing kernel collocation method (RKCM). To our understanding, little previous works exist on the implementation of nonlinear iterative solution procedure for the problems mentioned, especially when using the collocation methods. As RKCM has become one of the popular meshfree strong-form methods in solving the problems of concern, the apparent lack of existing nonlinear iterative procedure has given rise to the motivation of the present study. Furthermore, its application can be extended to problems involving strong nonlinearity. In this study, the procedures for conducting the quasi-Newton and Newton iteration schemes will be presented. The effects of various parameters appearing in the RKCM on the convergence characteristics of nonlinear analysis will be studied in detail.

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Title: XBraid: A Parallel Multi-Grid-In-Time Software Library

Author(s): Veselin Dobrev, Rob Falgout, Tzanio Kolev, Anders Petersson, Jacob Schroder, Ulrike Meier Yang, *LLNL*.

The need for parallel-in-time approaches, such as the parallel multigrid reduction in time (MGRIT) algorithm, is being driven by current trends in computer architectures where performance improvements are coming from greater parallelism, not faster clock speeds. This leads to a bottleneck for sequential time integration methods, because they lack parallelism in the time dimension. Thus, the ability to apply parallel-in-time approaches to application codes is of interest. MGRIT has been implemented in the software library XBraid. It is particularly well suited given its non-intrusiveness, which only requires users to wrap existing time stepping codes in the XBraid framework. In this presentation, we describe MGRIT and the corresponding software implementation XBraid. We also discuss the use of XBraid with a computational fluid dynamics application code and present performance results, which demonstrate a significant speedup if sufficient resources are available.

Title: Multi-Resolution Molecular Mechanics: A Unified and Consistent Framework for General Finite Element Shape Function

Author(s): Qingcheng Yang, Albert To, *U. Pittsburgh.*

We present a general mathematical framework for the newly proposed energy-based concurrent atomistic/continuum method Multiresolution Molecular Mechanics (MMM) [Q. Yang, E. Biyikli, and A. C. To, *Comput. Methods in Appl. Mech. Eng.* 258 (2013) 26-38]. The main features of the generalized framework are: (1) Consistency with the atomistic framework by directly employing the interatomic potential to calculate force and energy; (2) Simple procedure for analytically deriving the optimal summation rule for any given finite element shape function employed in the coarse-grained region. The procedure for obtaining the optimal summation rule is developed based on deriving and then fitting the atomic energy distribution within an element under the constraint of a given shape function. To validate the generalized framework, test problems including non-local harmonic and anharmonic models undergoing tensile, shear and bending deformations will be solved using linear, bilinear and quadratic elements, respectively. Results obtained using the proposed optimal summation rules for the different element types will be compared with Gauss quadrature for accuracy. Through error structure analyses, it is found that the proposed summation rule always outperforms Gauss quadrature, even when the latter employs more quadrature points than the former. It is argued that widely-used numerical quadrature techniques such as Gauss quadrature are not optimal for coarse-grained atomic energy approximation because they do not account for the discrete nature of the atoms. In contrast, the present summation rule is derived consistently from the underlying atomic energy distribution, and thus has better accuracy and smaller computational cost. [1] Q. Yang, A. C. To, Multiresolution molecular mechanics: A unified and consistent framework for general finite element shape functions, *Computer methods in applied mechanics and engineering*, 283 (2015) 384-418. [2] E.B. Tadmor, M. Ortiz, R. Phillips, Quasicontinuum analysis of defects in solids, *Philosophical Magazine A*, 73 (1996) 1529-1563 [3] J. Knap, M. Ortiz, An analysis of the quasicontinuum method, *Journal of the Mechanics and Physics of Solids*, 49 (2001) 1899-1923

Title: Enhancing Sparsity by Changing the Measure

Author(s): Xiu Yang, Huan Lei, Ramakrishna Tipireddy, Nathan Baker, *Pacific Northwest Nat'l. Lab.*;
Guang Lin, *Purdue U.*

Compressive sensing based uncertainty quantification method attracts many attentions in recent years. The capability of obtaining accurate global approximation, e.g., gPC, with a few sampling points makes this method suitable for complex systems with sparse representation. However, for high dimensional problems, the number of basis functions can be enormous even in a low order expansion, hence the number of samples to enable an accurate approximation is large. We aim to find a new set of random variables through linear/nonlinear mapping such that the representation of the quantity of interest is much sparser with new basis functions associated with the new random variables. At the same time we keep the property of the measurement matrix (e.g., mutual coherence) almost unchanged, hence the number of samples for an accurate approximation decreases. In other words, given a fixed number of samples, the new method yields a more accurate approximation due to the enhancement of the sparsity. We will demonstrate the efficiency of the new method with applications in stochastic partial differential equations and bio-molecular systems.

Title: Reduced Order Modeling for Vortex-Induced Vibration in Frequency Domain

Author(s): Weigang Yao, Rajeev K Jaiman, *Nat'l. U. Singapore.*

Vortex-Induced Vibration (VIV) is a self-limiting oscillation induced by nonlinear coupled flow-structural instability in the form of vortex shedding around vibrating body. In VIV, 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 to the value of frequency of the another system (e.g., vibrating structure). It constitutes an interesting problem for the numerical and mathematical modeling and can have a significant impact in the systems used in aerospace, ocean, and offshore engineering. Oscillating cylinder laterally in a free stream can form a great variety of vortex wake modes that have a profound role on the performance of structural dynamics and flow behavior. 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 nonlinear resonance shift. For sufficiently large amplitude, the wake is significantly perturbed and forced to move through the strong inertial coupling at the natural resonating frequency of the oscillating structure. The state-of-art CFD-based VIV simulation is less attractive in the scenarios of industrial routine analysis and multidisciplinary design optimization (MDO). Time domain simulation has to cover transient regime to achieve stationary periodic oscillation whereas its frequency counterpart only computes the periodic part and avoids any transient solution process. Therefore it is more efficient, when only the periodic part is of interest. Present work aims to develop an efficient and fast reduced-order model for lock-in VIV in frequency domain. Full CFD based Harmonic Balance (HB) method with frequency updating algorithm [1] is adopted to generate solutions at handful lock-in conditions (e.g., amplitude and Strouhal number). Flow modes can be extracted from the sample solutions by Proper Orthogonal Decomposition (POD) analysis. Solutions at other different lock-in conditions will be reconstructed from dominate flow modes, which are collected by truncating POD modes. To begin with, the reconstruction is achieved by interpolating modal coefficients at samples with two variables polynomial, which can be extended to the method for multi-variables interpolation. The contribution of present work is to develop a novel frequency updating algorithm [1] and enable CFD based HB solver to generate lock-in VIV solutions. The proposed method will be validated with our 2D freely vibrating cylinder VIV data. References [1] W.Yao et al, "Prediction of Transonic Limit Cycle Oscillations using an Aeroelastic Harmonic Balance Method", AIAA 2014-2310, submitted to AIAA Journal 2014, (minor revision).

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Title: A Coupled Rainfall-Runoff/River Flow Model for the Ohio River

Author(s): Mariah Yaufman, Cody Allison, Taylor Ross, Ethan Kubatko, *Ohio State U.*

In this talk, we describe the development and application of a coupled rainfall-runoff/river flow model for forecasting stage height and discharge for the Ohio River. This forecasting tool makes use of a discontinuous Galerkin method for solving the Saint Venant equations, which include lateral inflow source terms due to rainfall events occurring over the Ohio River watershed. We highlight some of the challenges involved in modeling the various rainfall-runoff processes (e.g., evapotranspiration, infiltration, etc.) and discuss the various data sets incorporated into the model, including detailed cross-sectional data for the Ohio River obtained from the US Army Corps of Engineers, topographic data generated from NASA's Shuttle Radar Topography Mission (SRTM) and land use/land cover data from the US Geologic Survey. The model is verified in a simplified setting against a set of analytic test cases and validated in a series of hindcasts that make use of historical rainfall and river gage data.

Title: Development and Validation of a Mesh Movement Framework for Finite-Element Simulation of Flow Beneath Ice Shelves

Author(s): Benjamin Yeager, Matthew Piggott, *Imperial College London*; Paul Holland, *British Antarctic Survey*.

The Antarctic Ice Sheet can be divided into two sections: the relatively stable East Antarctic Ice Sheet, grounded mainly above sea-level, and the West Antarctic Ice Sheet, which is grounded mainly below sea-level, making it vulnerable to collapse due to melting at its ocean boundary. The West Antarctic Ice Sheet contains enough ice to raise the global average sea level by 4m, and it is drained to the ocean by a number of glaciers that terminate in large, floating ice shelves. Melting at the ice-ocean interface of the fastest-moving glaciers is driven by the intrusion of warm deep-water which melts the ice at the grounding line of the glacier, resulting in a warm, buoyant meltwater plume that rises along the underside of the ice shelf. Uneven melting on the underside of the ice shelf leads to the development of channels and terraces in the ice, which affect the hydrodynamics of the buoyant plume, and in turn, the distribution of melting and refreezing. Here, we present the development of a mesh movement framework for finite element models, with the capability to handle moving domain boundaries and to focus resolution in important regions, such as those with sharp solution gradients. We then apply the framework to several test cases in order to demonstrate its ability to help capture the complex feedbacks between ice shelf geometry and sub-shelf hydro- and thermodynamics.

Title: Multi-Objective Optimization for Concrete Barrier Based on RBF Model

Author(s): Hanfeng Yin, Guilin Wen, Youxie Xiao, *Hunan U.*; Howie Fang, *U. North Carolina* .

At present, concrete barrier is one of most widely used guardrail systems for protecting the occupant safety of errant vehicle on the motorways. The performance of the concrete barrier is mainly influenced by its cross-sectional sizes. How to optimize the performance of concrete barrier is still a challenge for the roadside safety engineers due to the complicated relationship between the safety performance and the cross-sectional sizes. To solve this problem, a RBF-based multi-objective optimization method which jointly employs finite element analysis (FEA), RBF metamodeling technique and non-dominated sorting genetic algorithm-II (NSGA-II) was developed and used for optimizing a concrete barrier in this paper. The performance of the concrete barrier was evaluated by the criteria of the manual for assessment of safety hardware (MASH). In the optimization process, the RBF models of the objectives and constraints were constructed based on the FEA results of the samples generated by full factorial design method. Then, the NSGA-II was used to obtain the optimal designs of the concrete barrier by invoking those RBF models rather than invoking the FEA code which usually has expensive computational cost. After simulating the impact between the vehicles and the optimal concrete barrier, the results showed that the performance of the barrier was highly improved by comparing with its original design.

Title: In-Grid Spring Analysis of Full Spacer Grids with H-Type Springs

Author(s): JaeYong Kim, KyungHo Yoon, YoungHo Lee, KangHee Lee, HyungKyu Kim, HeungSeok Kang, *KAERI*.

A C-E(Combustion Engineering) type nuclear fuel assembly is composed with a top end piece(TEP), a bottom end piece(BEP), 4 guide tubes(GTs), a instrumentation tube(IT), 11 spacer grids(SGs), and several fuel rods. It has an outer flow passage which is located among nuclear fuel rods to exchange the central heat to coolant. In the dual-cooled fuel (called 'DUO') rod, an inner flow passage as well as an outer one is used not only to enhance the fuel safety but to achieve a power uprating through the decreasing fuel center temperature and increasing the heat transfer area between fuel and coolant. As a result, the diameter of a dual-cooled fuel becomes 1.6 times bigger than a conventional solid fuel and the gap between an annular fuel and spacer grid's straps is narrowed. So to form the supports (such as springs and dimples) within a cell is challenging problem in DUO[1]. Several types of springs have been invented for DUO rods. In this paper, numerical analysis models, analysis process, and analysis results were described for design and a spring characteristic analysis of one of them, a modified H type spring[2]. The finite element (FE) model for an in-grid spring characteristic analysis was established with special element density, which was determined to satisfy that the difference of the results for unit cell spring characteristic analysis and test was within 5 %. The analysis process was composed of two steps. As the first step, a spring back analysis was performed to simulate the springs to apply initial spring force to the fuel rods when the springs were deformed at the initial interference value. Following this step, a spring was deformed to measure the P- δ characteristic graph. This analysis method is verified by comparing the analysis results with the spring characteristic test results. Finally, the effect of position of a loading cell and the size of spacer grids are studied by this valuable analysis method. 1. H.K. Kim, J.Y. Kim, K.H. Yoon, 2011, Mechanical design issues and resolutions of a dual cooled fuel for OPR-1000, Nucl. Eng. Des. 241, 2119-2127 2. J.Y. Kim, K.H. Yoon, H.K. Kim, S.H. Ko, 2011, Modified H type spring design for dual cooled fuel rods, Proceedings of the Korean Nuclear Society Autumn Meeting

Title: Modeling of Contact and Non-Local Friction in a Peridynamic Framework

Author(s): Jason York, John Foster, *UT Austin*.

Key words: peridynamics, nonlocal, contact mechanics, frictional contact Contact problems representing the interaction of deformable bodies are frequently encountered and are vastly important in many physical applications. The inclusion of friction resulting from such contact generates an additional set of unique challenges. It is perceived that classical friction formulations, such as Coulomb's law, are only applicable to specific simplified cases. In response to the limitations of classical friction laws, nonlocal formulations [1] have been proposed to further describe observed friction phenomena. Nonlocality provides distinct advantages to a classical local formulation in its relation to the actual physical description of frictional contact. As the effects of friction relative to many physical processes are generally considered to be due to contact with a non-smooth surface, nonlocality may provide a more realistically homogenized representation. Additionally, normal contact pressures may be more accurately described, as they are distributed over asperities on non-smooth contact surfaces. Peridynamics [2] is an emerging nonlocal continuum formulation with growing applications, and strong potential in modeling material failure. This work will demonstrate the implementation of a contact model and resulting nonlocal friction in a peridynamic framework, impacting modeling capabilities such as fracture surface interactions. The resulting model is compared against classical contact problems for verification. REFERENCES [1] J.T. Oden, E.B. Pires, Nonlocal and nonlinear friction laws and variational principles for contact problems in elasticity. *Journal of Applied Mechanics*. 50, 67-76, (1983). [2] S. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari. Peridynamic states and constitutive modeling. *Journal of Elasticity*. 88, 151-184, (2007).

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Title: Unsteady Behavior of Cavitation Bubbles and Induced Shock Waves

Author(s): Hiroaki Yoshimura, Taro Miyazaki, *Waseda U.*

We will study unsteady phenomena such as rebound behavior of growth-collapse of cavitation bubbles with the induced shock wave. First, we will show some experimental results observed in bubble dynamics and will develop stochastic Rayleigh-Plesset equations. Second, we will study the unsteady behavior of the induced shock wave propagation from the collapse of a bubble and then we will estimate the impact pressure associated with the shock wave by numerical analysis.

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Title: Characterization of Fracture Properties of Non-Linear, Inelastic Paving Mixtures Using an Integrated Experimental-Computational Approach

Author(s): Taesun You, Yong-Rak Kim, *U. Nebraska.*

This paper presents characterization of fracture properties of nonlinear-inelastic paving mixtures using an integrated experimental-computational approach. Three-dimensional finite element model with cohesive zones is used to simulate a semicircular bending test where nonlinear viscoelastic and viscoplastic material behavior are considered in addition to cohesive zone fracture process. A series of laboratory tests are performed, and the test results are integrated with the three-dimensional finite element modeling to identify deformation characteristics such as the linear viscoelastic, nonlinear viscoelastic, and viscoplastic properties and fracture properties that are represented by the rate-dependent cohesive zone law. Pavement structure modeling is then performed to further investigate the effects of the individual energy dissipation sources of the mixtures on structural performance and to provide a better understanding of failure mechanisms in roadway design.

Title: Quasi-Linear RKPM and Its Application to Large Deformation and Fragmentation Modeling

Author(s): Edouard Yreux, J. S. Chen, *UC San Diego*.

RKPM relies on polynomial reproducing conditions to yield desired accuracy and convergence properties, but requires appropriate kernel support coverage of neighboring particles to circumvent singularity of the moment matrix when constructing approximation functions with order of approximation greater than zero. In this work, a quasi-linear RKPM formulation is proposed. Additional sampling points are used to evaluate the polynomial basis functions and construct an unconditionally nonsingular moment matrix without restriction to the minimal kernel support, while introducing controllable error in the linear field and preserving exact constant field reproduction. This approach provides a robust framework to enhance the accuracy of RKPM simulations at a very minimal computational cost, yet avoids numerical instabilities arising from insufficient kernel support coverage.

Title: Virtual Intraoperative Cholangiogram Using WebCL

Author(s): Doga Demirel, Alexander Yu, tansel halic, *U. Central Arkansas*; Sinan Kockara, .

We design and develop a virtual intraoperative cholangiogram using WebCL. Intraoperative cholangiogram (IOC) is a X-Ray based imaging procedure that is frequently used to identify the problematic pathological and physiological conditions during the surgical procedure particularly in cholecystectomy. In IOC, special dye is injected in the region of interest (e.g. bile ducts) to be able to highlight that with high-contrast on the X-Ray scanned image. We propose a WebCL algorithm to generate the virtual X-Ray images to simulate the IOC procedure. The virtual X-Ray images are computed based on Beer-Lambert attenuation law which is used to model the radiation absorption of emitted X-rays colliding the tissue structures or bones. In this model, the virtual rays will be emitted from a source to a 3D scene composed of triangles. The exact contact points of each ray will be determined to find the ray travel distance. Each emitted ray is attenuated at any contact on its path. The total attenuation on ray trajectory specifies X-ray emissivity of specimen under the exposed radiation. The entire procedure requires multi-pass algorithm and will have three phases; (1) computation of the total distance traveled by each ray within 3D models, (2) Augmentation of all computed distances with their corresponding attenuation cofactor for each object and (3) generation of the final gray-scale X-Ray image where injecting dye shows high contrast. All these steps are computation intensive and require real-time execution rates for the simulation of virtual IOC. WebCL, heterogeneous computing platform for web, is used for parallelization of each step in order to speed-up execution. The entire procedure is performed on the GPU of the web-client hardware. In this study, we present our multi-pass algorithm details and performance results on multiple devices with diverse computing capabilities.

Title: Towards Efficient Simulation of Unsteady Incompressible Flows Using Dual-Time Stepping
CPR-DG Methods on Unstructured Moving Grids

Author(s): Meilin Yu, Lai Wang, *U. Maryland.*

Accurate, robust and efficient simulation of unsteady incompressible flows is essential in many engineering applications, e.g., those in biological engineering and wind/hydro energy harvesting. Usually, these unsteady flows feature local flow separation with elaborate vortical structures around moving/deformable geometry. The high-order accurate arbitrary Lagrangian-Eulerian (ALE) numerical methods, capable of cost-effectively capturing tiny flow structures with low numerical dissipation, are desirable in the simulation of the vortex-dominated flows over moving/deformable boundaries as aforementioned. Conventionally, the SIMPLE-type or projection methods are used to solve unsteady incompressible flows. However, these methods suffer from inherent drawbacks. Firstly, they cannot be efficiently extended to the framework of modern high-order methods, e.g., discontinuous Galerkin (DG), flux reconstruction / correction procedure via reconstruction (FR/CPR), especially in the presence of moving boundaries. Secondly, existing computational techniques developed for compressible flows cannot be easily carried over to the simulation of incompressible flows. To facilitate the implementation of high-order methods in unsteady incompressible flow simulation, an artificial compressibility formulation and, correspondingly, a dual-time stepping procedure are used to reformulate the unsteady flow simulation problems. Specifically, an artificial pressure variation term with respect to the pseudo time is augmented to the continuity equation to create a new eigen-system of the governing equations. The CPR-DG formulation is used in the spatial discretization. The time derivative is discretized using the backward differentiation formulation. After that, at each physical time, an implicit pseudo-time integration system is formed, and then solved using a restarted GMRES method. Since the ALE formulation is adopted to handle moving grids, the Geometric Conservation Law (GCL) will be carefully examined in the dual-time stepping framework to remove conservation errors due to grid movement. After the development, the solver will be verified and validated using benchmark cases in the simulation of incompressible flows. This work will further advance the numerical simulation techniques for unsteady incompressible flows by using the CPR-DG formulation on moving grids with dual-time stepping.

Title: Mechanics of Structure Genome

Author(s): Wenbin Yu, *Purdue U.*

A new concept, Structure Genome (SG), is proposed to fill the gap between materials genome and structural analysis and unify structural mechanics and micromechanics. SG is defined as the basic building block of the structure connecting materials to structures and the mechanics of SG governs the necessary information to bridge materials genome and structural analysis. Mechanics of SG can be used to construct efficient yet high-fidelity constitutive models for composite structures over multiple length scales. The variational asymptotic method is used to mathematically decouple the constitutive modeling from the structural analysis. A general-purpose computer code called SwiftComp is developed to implement the mechanics of Structure Genome along with a few examples to demonstrate its application. Mechanics of SG presented in this paper enables a multiscale constitutive modeling approach with the following unique features: 1) Use SG to fill the gap between materials genome and structural analysis. Intellectually, SG enables us to view structural mechanics as an application of micromechanics. Technically, SG empowers us to systematically model complex buildup structures with heterogeneities of a length scale comparable to the smallest structural dimension. 2) Use VAM to avoid apriori assumptions commonly invoked in other approaches, providing the most mathematical rigor and the best engineering generality. 3) Decouple the original problem into two sets of analyses: a constitutive modeling and a structural analysis. This allows the structural analysis to be formulated exactly as a general (1D, 2D, or 3D) continuum, the analysis of which is readily available in commercial FEA software packages and confines all approximations to the constitutive modeling, the accuracy of which is guaranteed to be the best by VAM.

Title: Multi-Scale Modeling of Strength and Toughness of 3D IC Intermetallic Micro Bumps

Author(s): Chi-Hua Yu, Chih-Chuen Lin, Chuin-Shan Chen, *Nat'l. Taiwan U..*

A three-dimensional integrated circuit (3D IC) is a chip in which multiple layers of electronic components are vertically integrated. 3D IC is an IC design revolution and has a great potential to significantly improve chip performance. 3D IC relies on micro-bumps to connect the components. Thus, the structural integrity of micro-bumps plays a key role for 3D IC integration. The demands of high-performance 3D IC naturally lead to micro-bumps solely consisting of single-crystal intermetallic compounds (IMC). Thus, a comprehensive study of fracture strength and toughness of a single-crystal IMC becomes imperative. In this talk, we will present our recent multiscale modeling and simulation to predict fracture strength and toughness of single-crystal IMC at about 5 micron length scale through first principles density functional theory (DFT) and finite element method (FEM). Virtual crystal approximation in DFT is adopted to study crystallographic dependence of mechanical properties of Cu₆Sn₅, Ni doped Cu₆Sn₅ and Ni₃Sn₄ which appear during the growth process of dopant IMC. The calculated properties are used in FEM to study mechanical behavior of IMC micro-bumps. Numerical results are compared with experimental measurements from micro-pillar tests. The predictive methodology developed in this study will benefit semiconductor industries to design and manufacture a more reliable, durable, and stronger 3D IC.

Title: A Stabilized Explicit Scheme for Coupling Fluid-Structure Interactions

Author(s): Yue Yu, *Lehigh U.*

We develop a new stabilized explicit coupling partitioned scheme for the fluid-structure interaction problem, where the pressure and velocity are decoupled. Proper penalty terms are applied to control the variations at the interface. Using energy stability analysis, we show that the scheme is stable independent of the fluid-structure density ratio. Numerical examples are provided to show that although the penalty terms degrade the time accuracy, optimal accuracy is recovered by performing defect-correction subiterations.

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Title: Computational Modeling of the Spatially Coordinated Mechanosensing in Cell-Microenvironment Interactions

Author(s): Hongyan Yuan, *U. Rhode Island.*

Understanding the mechanical aspect of cell-microenvironment interactions is important to many biological and biomedical problems such as morphogenesis, tissue engineering, wound healing, and cancer metastasis. It is hypothesized that biological cells integrate and coordinate the molecular scale mechanotransduction events over the whole cell scale based on continuum mechanics principles, and interact with their mechanical microenvironment as a whole. In this work an extended finite element-based computational model is developed to explore this hypothesis in silico. In this model, continuum mechanics equations, reaction-diffusion equations, and rate equations are coupled together to model the feedback loops between mechanical stresses and biochemical signals, and to explore the emergence of cell shapes and micro-tissue morphologies.

Title: Automatic 3D Symmetric Clone Mesh Generation for Motor Designs

Author(s): Wei Yuan, Ravi Sundaram, Eric Lin, ANSYS.

Rotary electrical machines consist of moving parts and stationary parts separated by a very small band gap. Some of the moving and static parts have periodic structures in the rotational direction. In the transient simulation we apply a rigid body transformation on the mesh of the moving parts. Thus the relative positions of the moving region mesh and the stationary region mesh change in every time step. The computation of cogging torque is very sensitive to the mesh noise at the rotational time steps. It is critical in the motor designs to have these repeated structures be meshed identically to minimize the mesh noise. The typical field gradients in the motor designs are very high in the rotational direction and much lower in the axial direction. For efficient transient simulation, the elements need to be stretched in the axial direction and compressed in the rotational direction. This paper introduces an automatic 3D multi-region mesh generation method. The motor model is divided in the radial direction into static, moving and band regions. Within each region, it is further separated into multiple sections along the axial direction based on geometric features such as: clone section, symmetric section, sweep section and skewed section. In each section, the meshing process is tailored to the application's needs. For the section with periodic rotational regions, one local region is defined as the master region, and the others are defined as slave regions. A volume mesh is generated only for the master region, then copied and pasted to the slave regions to guarantee identical meshes in each region. In a symmetric region, the mesh is generated in the master region, and then mirrored to the slave region to get a symmetric mesh. In the sweep region, a uniform 2D mesh is generated first, and then extruded in the axial direction to obtain the optimized volume mesh. In the skewed region, the regular 3D mesh generation method will be applied. The regional static mesh and the moving mesh are obtained by assembling the meshes from different sections. The final conformal mesh is generated by combining the meshes from all three regions. Examples will be presented to show this new mesh generation method is efficient and accurate in practical motor designs

Title: An Extended Finite-Element Algorithm for the Fracture Analysis of Metal Matrix Composites with Realistic SiC Particle Geometries Obtained from X-Ray Synchrotron Tomography Data

Author(s): Rui Yuan, Sudhanshu S. Singh, Nikhilesh Chawla, Jay Oswald, *ASU*.

We present an extended finite element method (XFEM) for modeling fracture initiation in metal matrix composites. The complex microstructure of SiC particles in an Al alloy matrix is represented implicitly by a level set field initialized from X-ray tomography measurements. In the simulations, the aluminum phase is modeled with a J2 plasticity model with nonlinear hardening, while the SiC reinforcement particles are treated as brittle and elastic. A Weibull fracture model is implemented for the prediction of cleavage fracture in the brittle particles. In this analysis, both weak and strong discontinuities are embedded within the approximated solution at particle boundaries and fracture surface respectively, through the XFEM, where oct-tree mesh refinement is used to enable satisfactory resolution of the complex particle surfaces. The accuracy of the method is demonstrated through comparison of particle fracture measured through 4D in-situ X-ray synchrotron tomography experimental measurements conducted during the fracture process.

Title: Stabilizing Large-Deformation Elastic-Plastic Analysis of Cracked Model with Partitioned Coupling Method

Author(s): Yasunori Yusa, Shinobu Yoshimura, *U. Tokyo.*

When a cracked structure is subjected to excessive loading such as a strong earthquake, the crack tip vicinity becomes a state of large-strain plasticity. However a most portion of the structure far from the crack can stay as an elastic body. For such a problem, we have studied a partitioned coupling method [1], in which the interaction between a cracked local domain and an uncracked global domain is analyzed. The two domains are analyzed separately and iteratively with assumed boundary conditions on the global-local interface. The boundary conditions are updated at every iteration step by an iterative solution technique. In our previous study [2], a large-deformation elastic-plastic problem of a notched specimen model was analyzed with the partitioned coupling method. The local domain with a notch was modeled as a large-deformation elastic-plastic body, whereas the global one was done as a large-deformation elastic body. The analysis was terminated abnormally at an incremental step because of a singular stiffness matrix. In this presentation, the large-deformation elastic-plastic analysis with the partitioned coupling method is stabilized with an improved iterative solution technique. [1] Yusa, Y. and Yoshimura, S. Speedup of elastic-plastic analysis of large-scale model with crack using partitioned coupling method with subcycling technique. *Computer Modeling in Engineering and Sciences*, vol. 99, no. 1, pp. 87-104, 2014. [2] Yusa, Y. and Yoshimura, S. Analysis of cracked model under finite-strain elastoplasticity using partitioned coupling method. 11th World Congress on Computational Mechanics, 5th European Conference on Computational Mechanics, and 6th European Conference on Computational Fluid Dynamics, Barcelona, Spain, July 2014.

Title: Neural Networks for Computational Homogenization and Optimization of Hyperelastic Heterogeneous Materials

Author(s): Julien Yvonnet, Ba Anh Le, Qi-Chang He, *U. Paris-Est.*

In this work, a decoupled computational homogenization method for nonlinear elastic materials is proposed using Neural Networks (NN) [1]. In this method, the effective potential is represented as a response surface parameterized by the macroscopic strains and some microstructural parameters. The discrete values of the effective potential are computed by FEM [2] through random sampling in the parameter space, and NN are used to approximate the surface response [3] and to derive the macroscopic stress and tangent tensor components. We show through several numerical convergence analyses that smooth functions can be efficiently evaluated in parameter spaces with dimension up to 10, allowing considering 3D Representative Volume Elements (RVE) and an explicit dependence of the effective behavior on microstructural parameters like volume fraction. The advantage of this feature is discussed for design of heterogeneous materials with optimized properties. REFERENCES [1] B.A. Le, J. Yvonnet, Q.-C. He, Computational homogenization of nonlinear elastic media using Neural Networks, submitted. [2] J. Yvonnet, D. Gonzalez, Q.-C. He, Numerically explicit potentials for the homogenization of nonlinear elastic heterogeneous materials, *Comput. Methods Appl. Mech. Eng.*, 198:2723-2737 (2009). [3] S. Manzhos, K. Yamashita, T. Carrington, Fitting sparse multidimensional data with low dimensional terms, *Comput. Phys. Commun.*, 180:2002-2012 (2009).

Title: Unsteady CFD Shape Optimization Using High-Order Discontinuous Galerkin Finite-Element Methods

Author(s): Matthew Zahr, *Stanford U.*; Per-Olof Persson, *UC Berkeley*.

PDE-constrained optimization has become an essential tool in the design of steady-state fluid systems, but is less commonly used for unsteady problems, particularly with the nonlinear, compressible, Navier-Stokes equations as the constraining PDE. However, there is a large-class of problems that are inherently unsteady, such as flow past airfoils at a high angle of attack and flow through wind farms, that would benefit from numerical optimization. In this work, a framework for shape optimization for unsteady, viscous CFD problems is developed. Since the optimization functionals require reliable accuracy in the computed output quantities and their gradients, the governing equations are discretized using a high-order discontinuous Galerkin (DG) spatial discretization and high-order temporal discretization. In the case of unsteady shape optimization, the geometry of interest will in general be evolving with time, resulting in a deforming fluid domain. This is handled by a high-order accurate mapping-based Arbitrary Lagrangian-Eulerian (ALE) approach. The corresponding Geometric Conservation Law (GCL) is satisfied by solving an auxiliary set of ODEs [1]. The deformation of the body and the surrounding high-order fluid mesh is performed using free-form deformation [2]. The fully-discrete adjoint method is used to compute gradients of CFD output functionals with respect to the shape parameters. The proposed high-order unsteady CFD optimization framework will be demonstrated on viscous CFD test problems. A comparison will be made between low-order and high-order spatial discretizations. Future work will focus on reducing the relatively high computational cost associated with unsteady optimization for CFD problems by using a reduced-order model as a surrogate for the high-order DG equations. The benefits of using a high-order discretization will be preserved by considering a globally-convergent sequence of such reduced optimization problems. [1] Persson, P.-O., Bonet, J., and Peraire, J., "Discontinuous Galerkin solution of the Navier-Stokes equations on deformable domains," *Computer Methods in Applied Mechanics and Engineering*, Vol. 198, No. 17, 2009, pp. 1585–1595. [2] Sederberg, T. W. and Parry, S. R., "Free-form deformation of solid geometric models," *ACM SIGGRAPH computer graphics*, Vol. 20, ACM, 1986, pp. 151–160.

Title: Computational Analysis of Energy Distribution of Coupled Blood Flow and Arterial Deformation

Author(s): Rana Zakerzadeh, Paolo Zunino, *U. Pittsburgh.*

Considering arterial wall as an elastic structure is a common assumption in Fluid Structure Interaction simulations. However; it neglects realistic arterial wall model. In reality, arterial wall like other soft tissues is viscoelastic and it shows poroelastic behavior as well. The present study attempts to investigate the effect of both poroelasticity and tissue viscoelasticity on fluid-structure interaction in arteries and analyze the role of extracellular fluid flow in the apparent viscoelastic behavior of the arterial wall. We also study the energy exchange in the interaction between the blood flow and the arterial wall to investigate the distribution and dissipation of the energy delivered to the artery during one heart cycle. To this aim, we develop a computational method that allows us to simulate the propagation of pressure waves and the related arterial wall deformation into an arterial segment. Blood is modeled as an incompressible, viscous, Newtonian fluid using the Navier-Stokes equations and the arterial wall consists of a thick material which accounts for the media and the adventitia. This thick layer is modeled using different constitutive models; namely elastic, viscoelastic and poroelastic. Viscoelastic mechanical properties of vessel walls were modeled by utilizing a simple linearly viscoelastic model which is based on Kelvin-Voigt viscoelasticity. For poroelastic case, the arterial wall is considered as Biot system that describes the mechanical behavior of a homogeneous and isotropic elastic skeleton, and connecting pores filled with fluid. We assume that the fluid flow through the pores is modeled using the Darcy equation. In order to approximate this problem, we develop a partitioned, loosely coupled finite element solver based on weak enforcement of interface conditions using Nitsche's method that allows us to independently solve the equations at each time step. Namely, structure mechanics, the intramural filtration and the blood flow problem are solved separately at each time step. The conservation of the energy principle has been applied systematically to the arteries to assess energy exchange between different compartments of the model. Energy estimation for each constitutive model of the arterial wall is derived from weak formulation for the coupled problem, and numerical tests are performed using physiological parameters to support its accuracy.

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Title: Open-Source Software for Automation of Verification, Validation, and Uncertainty Quantification of Codes in Computational Mechanics

Author(s): James Courtney, Kaveh Zamani, Fabian Bombardelli, *UC Davis*.

Recently developed software is presented for automated Verification and Validation (V&V) and Uncertainty Quantification (UQ) for engineering codes that approximate Partial Differential Equations (PDEs). The code post-processes model results to produce V&V and UQ information. This information can be used to assess model performance. Automated information on code performance can allow for a systematic methodology to assess the quality of model approximations. The software implements common and accepted code verification schemes. The software uses the Method of Manufactured Solutions (MMS), the Method of Exact Solution (MES), Cross-Code Verification, and Richardson Extrapolation (RE) for solution (calculation) verification. It also includes common statistical measures that can be used for model skill assessment. Complete RE can be conducted for complex geometries by implementing high-order non-oscillating numerical interpolation schemes within the software. Model approximation uncertainty is quantified by calculating lower and upper bounds of numerical error from the RE results. The software is also able to calculate the Grid Convergence Index (GCI), and to handle adaptive meshes and models that implement mixed order schemes. Four examples are provided to demonstrate the use of the software for code and solution verification, model validation and uncertainty quantification. The software is used for code verification of a mixed-order compact difference heat transport solver; the solution verification of a 2D shallow-water-wave solver for tidal flow modeling in estuaries; the model validation of a two-phase flow computation in a hydraulic jump compared to experimental data; and numerical uncertainty quantification for 3D CFD modeling of the flow patterns in a Gust erosion chamber.

Title: Association of Intraluminal Thrombus and Hemodynamic Factors for Abdominal Aortic Aneurysm Expansion

Author(s): Byron Zambrano, Hamidreza Gharahi, Jongeun Choi, Chae-Young Lim, Farhad Jaber, Seungik Baek, *Michigan State U.*; Whal Lee, *Seoul Nat'l. U. Hospital.*

Abdominal aortic aneurysm (AAA) is the focal dilatation of the aorta at the abdominal level. Its rupture has been linked to a high mortality rate. Among multiple factors that affect AAA growth, the intraluminal thrombus (ILT) and hemodynamic conditions are believed to play important roles. Hemodynamic forces imposed on the arterial wall as wall shear stress (WSS) have an impact on the mechano-hemostasis of the arterial wall. In fact, a negative correlation between WSS and AAA expansion have been suggested. This relationship, however, is not that simple since ILT is found in 75% of AAA detected. Once ILT is formed, hemodynamic conditions would not interact directly with the arterial wall and instead, it would regulated the thrombus accumulation which in turn would interact with the AAA expansion. Despite the importance of studying these parameters, most of the studies focus their attention on two of these three important factors. Therefore, the present study used longitudinal CT images of 14 different patients to study the association between changes of hemodynamics, ILT and AAA growth. Geometric parameters as AAA and ILT volume rates were used to represent changes in ILT accumulation and AAA growth respectively and different hemodynamic variables as: oscillatory shear index (OSI), wall shear stress (WSS), near wall residence time (NWRS) and platelet activation potential (PLAP) were used to represent different hemodynamic factors impacting either AAA growth or ILT accumulation. Results showed that wall shear stress on AAAs without ILT showed to be higher then those that developed an accumulation. On AAA that developed an ILT accumulation, ILT showed initially to accumulate at a localized region of maximum diameter and spread to neighboring regions while ILT continued to thicken at covered areas. This accumulation rate showed to be same as the AAA expansion rate. On these patients, the diameter-expansion relationship was not as strong as it was for those AAAs that did not develop thrombus. Results suggest that a lower wall shear stress may be necessary for the thrombus to accumulate. It also suggests that once ILT forms, it can promote higher expansion rates, increasing probability for it to rupture and making the AAA growth rate prediction-using diameter unreliable.

Title: Parallel RBF Kernel-Based Stochastic Collocation for Large-Scale Random PDEs

Author(s): Peter Zaspel, Michael Griebel, *U. Bonn.*

Our aim is to solve large-scale uncertainty quantification problems in a high-order convergent, scaling, parallel and optimal complexity fashion. To this end, we recently introduced the radial basis function (RBF) kernel-based stochastic collocation method. This non-intrusive approach combines high-order algebraic or even exponential convergence rates of spectral (sparse) tensor-product methods with optimal preasymptotic convergence of kriging and the profound stochastic framework of Gaussian process regression. The new method uses Lagrange bases from special reproducing kernel Hilbert spaces for approximation. Those Hilbert spaces are constructed from RBFs. Current applications are (elliptic) model problems and incompressible two-phase flows. We are able to show up to exponential convergence for model problems with high smoothness. For problems with low-smoothness, algebraic convergence rates can be given. A small error in the preasymptotic regime is always achieved. Convergence results of (quasi-)Monte Carlo and (sparse) spectral tensor-product approaches are often clearly outperformed. We are further able to present an empirical error coupling analysis. Performance measurements show that we can solve and analyze large-scale two-phase flow problems within a few hours. This excellent preasymptotic runtime becomes possible by parallelizing all relevant numerical methods, including a two-phase flow solver, iterative dense linear algebra solvers and all parts of the stochastic collocation on graphics processing units (GPUs). Most approaches scale across clusters of GPUs. Optimal complexity and profound speedups are achieved by preconditioning of iterative sparse and dense linear solvers. Dense linear systems from interpolation are preconditioned with a localized restricted additive Schwarz method. Thereby, a new perfectly scalable preconditioner on multi-GPU clusters is constructed. Elliptic problems are solved with a newly implemented optimal Ruge-Stüben algebraic multigrid method. It uses CPU-based C/F splittings and parallelizes all remaining parts of the setup and solve phase on one GPU. The curse of dimensionality is weakened or even broken for problems with fast decaying output covariance spectrum. To this end, anisotropic RBF kernel-based stochastic collocation is introduced. Optimal weights for two-phase flow problems are approximated by a Karhunen-Loève expansion of the solution flow field, which requires to solve a large-scale dense eigenvalue problem. Greedy optimization is used for optimal sampling in anisotropic space. Numerical experiments give profound (pre-)asymptotic results for elliptic and two-phase flow problems. Overall, we will be able to show that a combined effort of optimal numerical methods and parallel implementations allows to solve even large-scale uncertainty quantification problems in a small amount of time.

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Title: Analysis of the Mechanical Response of Biomimetic Materials with Highly Oriented Microstructures Through 3D Printing, Mechanical Testing and Modeling

Author(s): Enrique Escobar, Chanhue Jeong, Pablo Zavattieri, *Purdue U.*; Lessa Grunenfelder, David Kisailus, *UC Riverside*.

Many biomineralized organisms have evolved highly oriented nanostructures to perform specific functions. One key example is the abrasion-resistant rod-like microstructure found in the radular teeth of Chitons (*Cryptochiton stelleri*), a large mollusk. The teeth consist of a soft core and a hard shell that is abrasion resistant under extreme mechanical loads with which they are subjected during the scraping process. Such remarkable mechanical properties are achieved through a hierarchical arrangement of nanostructured magnetite rods surrounded with alpha-chitin. We present a combined biomimetic approach in which designs were analyzed with additive manufacturing, experiments, analytical and computational models to gain insights into the abrasion resistance and toughness of rod-like microstructures. Staggered configurations of hard hexagonal rods surrounded by thin weak interfacial material were printed, and mechanically characterized with a cube-corner indenter. Experimental results demonstrate a higher contact resistance and stiffness for the staggered alignments compared to randomly distributed fibrous materials. Moreover, we reveal an optimal rod aspect ratio that lead to an increase in the site-specific properties measured by indentation. Anisotropy has a significant effect (up to 50%) on the Young's modulus in directions parallel and perpendicular to the longitudinal axis of the rods, and 30% on hardness and fracture toughness. Optical microscopy suggests that energy is dissipated in the form of median cracks when the load is parallel to the rods and lateral cracks when the load is perpendicular to the rods. Computational models suggest that inelastic deformation of the rods at early stages of indentation can vary the resistance to penetration. As such, we found that the mechanical behavior of the system is influenced by interfacial shear strain which influences the lateral load transfer and therefore the spread of damage. This new methodology can help to elucidate the evolutionary designs of biomineralized microstructures and understand the tolerance to fracture and damage of chiton radular teeth.

Title: Homogenization of Additive Manufactured Polymeric Foams with Spherical Cells

Author(s): Hamed Zeinalabedini, Pu Zhang, Mesut Kirca, ; Albert C. To, *Pittsburgh U.* .

Exciting progress in additive manufacturing (AM) technology, which enables fabrication of cellular structures such as highly complex lattice and porous structures, has stimulated the development of lightweight structural products with improved performance and increased functionality. However, conventional design and analysis tools lack the ability to optimize complex geometries efficiently and robustly. With this motivation, in this study, homogenized material models of open-cell polymeric foams with spherical cell architectures that are manufactured using AM technology are formulated through both experimental and numerical investigations, which in turn can be employed in a novel micromechanics based topology optimization algorithm [1] developed for the optimization of cellular structures. In this regard, for the purpose of generating computer aided drawing (CAD) data, which is mandatory for AM, randomly intersected spherical ensemble method [2] is employed. Several foam models with different porosities are generated and utilized in nonlinear finite element analyses (FEAs) to determine constitutive elastic constants. Plastic stress-strain data for the bulk AM material are obtained through static tensile tests in different loading directions and used in FEA as true stress-strain data. Homogenization is performed based on a quadratic form of the widely used Gibson and Ashby foam model that describes the Young's modulus, shear modulus, and yield strength of cellular structures in terms of relative density. Coefficients of the quadratic scaling laws are fitted by both FEA and experiments which are compared with each other. References [1] P. Zhang, J. Toman, Y. Yu, E. Biyikli, M. Kirca, M. Chmielus, and A. C. To. (2015) Efficient design-optimization of variable-density hexagonal cellular structure by additive manufacturing: Theory and validation, *J. Manuf. Sci. Eng.* 137(2), 021004. [2] A. To, J. Tao, M. Kirca, and L. Schalk (2011) Ligament and Joint Sizes Govern Softening in Nanoporous Aluminum, *Appl. Phys. Lett.*, 98(5), p. 051903.

Title: Computational Modeling of Collective Epithelial Cell Migration

Author(s): Xiaowei Zeng, Liqiang Lin, *UTSA*.

Cell migration plays an essential role in many physiological processes including morphogenesis, wound healing and tumor metastases. There are different modes of cell migration depending on the cell type and the context in which it is migrating. Cells can move as single entities or collectively through migration of cohesive cell groups. Although factors affecting migration of single cell are beginning to be understood, still little is known about motion when cells are in collective groups. In this presentation, we shall present our latest results on modeling and simulation of collective epithelial cell migration. The macroscale cell is modeled as soft materials and cell-cell interaction is governed by a recently developed interfacial bonding model. The polygonal shape of epithelial cells is generated using Voronoi tessellation techniques with an average size of 30 μm . We have developed and implemented a cohesive interface zone model and related computational algorithms for the described cell migration model. The simulation shows that the collective cell migration motion depends on different factors such as cell stiffness, the size of cohesive cells, cell-cell adhesion strength and substrate rigidities.

Title: A Variational Multi-Scale Approach for Transient Dynamics of Viscoelastic Materials Using Linear Tetrahedral Finite Elements

Author(s): Xianyi Zeng, Guglielmo Scovazzi, *Duke U.*

We present a variational multi scale (VMS) approach for transient dynamics of viscoelastic materials using piecewise linear tetrahedral elements. Our method uses a mixed formulation of piecewise linear approximations in both velocity and pressure. Standard Galerkin methods of this kind often suffer from instability in pressure, especially in the nearly incompressible limit. In our previous work [1], a VMS-approach is developed to stabilize the numerical scheme for isotropic elastic materials by writing the pressure equation in rate form. In this work, we extend the methodology to isotropic viscoelastic materials, seeing that most inelastic deformation in this category preserves the volume of the material. The latter fact implies that the time rate equation for pressure remains unchanged by including the viscoelastic model to the underlying hyperelastic models. We consider viscoelastic materials in both infinitesimal strain regime and in the finite strain regime. In particular, the linear viscoelastic effect is modeled by using the Prony series expansion of the relaxation function. And we introduce internal variables at the quadrature points of each element to keep track of the contribution of the stress history to the Cauchy stress in the current configuration. To demonstrate that the stabilized method does not depend on a specific model, we consider two extensions to finite strain viscoelastic materials. In the first model, we use the relaxation function as in the linear case, and follow the explicit integration method in [2] to update the internal variables from one time step to the next. In the second model, we use the multiplicative theory of viscoelastic materials in finite strain regime [3] by writing the deformation gradient as the product of an elastic one and an inelastic one. We demonstrate the second-order accuracy and improved stability of the proposed methods by extensive tests in 2D plain strain case and fully 3D problems. The presentation is concluded by the numerical simulation of the interaction between a blast wave and a gel-like solid that is modeled as viscoelastic material. [1] G. Scovazzi, B. Carnes, and X. Zeng. A stabilized method for transient solid dynamics of isotropic nearly incompressible elasticity with linear tetrahedral finite elements: a variational multiscale approach. (In preparation.) [2] J. C. Simo and T. J. R. Hughes. Computational Inelasticity. Springer, 2000. [3] S. Reese and S. Govindjee. A Theory of Finite Viscoelasticity and Numerical Aspects. Int. J. Solids Struct., 1998.

Title: A Smoothing Technique Based Beta Finite-Element Method and Its Application for Modeling Crystal Plasticity

Author(s): Wei Zeng, Guirong Liu, *U. Cincinnati*.

The smoothed finite element techniques were recently developed for various solid mechanics problems and working effectively with triangular or tetrahedral meshes which can be generated conveniently for complex geometries. In this work, the concept of smoothing technique based beta finite element method (betaFEM) is proposed. Smoothing domains generated from both edge-based (face-based for 3D) and node-based strain smoothing techniques are employed to construct a smoothed model. An adjustable parameter "beta" controls the portion of area of edge-based/face-based and node-based smoothing domains. In the context of elasticity, it is promising to find nearly exact solution in strain energy due to solution shifting by tuning the adjustable parameter, since the exact solution is bonded by the system constructed using NS-FEM and ES-FEM. A key aspect of the method is that it inherits the features of both NS-FEM and ES-FEM, such as ultra-accuracy, insensitivity to mesh quality or distortion, alleviation of volumetric locking, etc. Standard patch tests are likewise satisfied. After numerical investigation of accuracy and volumetric locking in elastic problems, the method is then performed to modeling rate-independent crystal plasticity problems. Numerical results attest its capabilities of treating plastic incompressibility and volumetric locking. The predictions of strain localization and shear band development show good agreement with literatures, which utilized some special elements such as Q1E4 elements, Q1/P0 elements or F-bar elements. The proposed method and algorithm are also implemented to simulate the mechanical behavior of polycrystalline aggregates through modeling the synthetic microstructure constructed by Voronoi tessellation technique. It is argued that β FEM is a viable alternative to standard FEM and possesses several advantages.

Title: Cell Responses to Rotational Nanoparticles

Author(s): Liuyang Zhang, *U. Georgia.*

Understanding and controlling the interaction of rotational nanoparticles (RNP) with cell is critical to the development of its biomedical applications. Here we perform dissipative particle dynamics simulations to analyze the rotation period, size, and coating pattern as the RNP interacts with the cell so as to provide novel design of drug delivery applications. It's shown that the rotational RNP is capable to intriguer local disturbance and promotes the cell translocation toward RNP. During the studies, we mainly focused on the translocation time required for RNP entering inside cell under various rotation periods as well as the interaction energy between coated RNP and cell. Through ligand pattern design on RNP, we could find a suitable nanoparticle candidate with a specific ligand coating pattern for drug delivery. We also find that channel-like RNP could connect the cells to form the network which facilitate the substances change between the cells. Our findings provide useful guidelines for the molecular design of patterned RNP for controllable interfaces and help establish qualitative rules for the organization and optimization of ligands for desired drug delivery.

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Title: A Multi-Scale Mechanobiological Model Considering the Structure and Interrelation of ECM Constituents in Aorta

Author(s): Katherine Zhang, *Boston U.*

The complex network structure of elastin and collagen extracellular matrix (ECM) forms the primary load-bearing component in the arterial wall. Pathogenesis of many cardiovascular diseases is associated with loss of organization and function of the ECM. However the interrelation of the function of collagen and elastin and the effect of ECM structural changes on vascular mechanics are not well understood. This talk will focus on our recent study on the interrelations of ECM constituents and how they contribute to the mechanical function of the arterial wall. Our recent study coupling mechanical loading and multi-photon imaging demonstrates an interesting sequential engagement of elastin and collagen fibers in response to mechanical loading. Our study also suggests that the elastin fibers are under tension and impart an intrinsic compressive stress on collagen. Such delicate interrelation between elastin and collagen is essential for an artery to function normally. Studies of the structural components and mechanics of arterial ECM generally focus on elastin and collagen while glycosaminoglycans (GAGs) are often neglected, most likely because of the relatively low content in arterial tissue. Our study also shows that GAGs play a role in engaging the elastin and collagen fibers in the arterial wall and thus indirectly affect the biomechanical function of arteries. Together these results provide a more comprehensive understanding of the mechanobiology of arteries. The structural information is incorporated into a mechanobiological constitutive model of ECM mechanics in order to provide a clinical relevant relationship between biomechanical integrity, biochemical composition stability, and microstructure of the ECM. A statistical mechanics based approach is adopted to determine the strain energy change accompanying deformation of a single fiber. A freely joined chain model is adopted to describe the possible configurations, thus entropy, of a fiber during tissue deformation. The fiber-level model is then incorporated into a tissue-level model by considering ECM fiber distribution function and adding fiber density. A multi-scale mechanobiological model that incorporates inter-molecular cross-linking, fiber distribution and fiber density is achieved for the description of tissue-level function.

Title: The Role of Connective Tissue in Skeletal Muscle Force Generation: A Multi-Scale Investigation

Author(s): Yantao Zhang, J.S. Chen, *UC San Diego*.

It's well known that the active force generation capability of skeletal muscle deteriorates with ageing. While the loss of mass in contractile component, the reduction in specific fiber tension or loss of motor units are possible reasons causing force reduction, they cannot explain the observed phenomenon where the decrease in force generation during eccentric contraction (lengthening) is much less than that in concentric contraction (shortening) [1]. In fact, experimental observations suggest (1) the skeletal muscle conserves the force generation capability in eccentric contraction with ageing, and (2) the stiffness in connective tissue increases with ageing [2]. This study provides a numerical investigation on how the stiffness of the connective tissue affects muscle force generation. The proposed numerical model is a honeycomb-like microstructure in the fiber level simulated by the pixel based meshfree method [3]. The numerical investigation reveals that the increased stiffness of connective tissue reduces the force generation capability in concentric contraction while increases the force generation capability in eccentric contraction. The proposed model provides a way to investigate into the micro-scales of skeletal muscle, and can also be easily extended to study other physiological changes due to ageing or diseases. [1] S. V. Brooks and J. A. Faulkner, "Isometric shortening and lengthening contractions of muscle fiber segments from adult and old mice," *Am. J. Physiol.*, vol. 267, pp. C507-C513, 1994. [2] Y. Gao, T. Y. Kostrominova, J. A. Faulkner and A. S. Wineman, "Age related changes in the mechanical properties of the epimysium in skeletal muscles of rats," *Journal of Biomechanics*, pp. 465-469, 2008. [3] J. S. Chen, S. Yoon and C. T. Wu, "Non-linear version of stabilized conforming nodal integration for Galerkin mesh-free methods," *International Journal for Numerical Methods in Engineering*, pp. 2587-2615, 2002.

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Title: A High-Order, 3D-Flow Solver for Compressible Viscous Flows on Coupled Rotating/Stationary Domains Using Spectral Difference Method and a Novel Sliding-Mesh Interface Approach

Author(s): Bin Zhang, Chunlei Liang, *George Washington U.*

This paper presents a newly developed 3D flow solver for compressible viscous flows on coupled rotating/stationary domains. The solver uses spectral difference method and a novel sliding-mesh interface approach. On the nonconforming sliding-mesh interfaces, the related variables are first projected to curved dynamic mortars to compute common fluxes, and then the common fluxes are projected back to the cell faces to ensure conservation. This novel 3D curved dynamic mortar approach is an extension of the previously reported approach for 2D simulations[1]. To verify the spatial order of accuracy of the solver, both inviscid and viscous flow cases are tested. It is shown that the solver with sliding-mesh interfaces preserves the high-order accuracy of the SD method. Meanwhile, the solver is found to be very efficient in terms of computational cost. This novel high-order solver with sliding-mesh interfaces can be applied to a wide range of problems, such as the aerodynamics of rotorcraft, wind turbines, and oscillating wing wind power generators, etc. [1] B. Zhang, C. Liang, A Simple, Efficient, High-Order Accurate Sliding-mesh Interface Approach to FR/CPR Method on Coupled Rotating and Stationary Domains, AIAA paper, 2015

Title: High-Order, Finite-Element Analysis of Boundary Layer Flows

Author(s): Alvin Zhang, Onkar Sahni, *RPI*.

Modeling of boundary layer flows requires careful approximations, especially for turbulent boundary layers. Making use of isotropic elements (in geometric shape or basis functions) puts an excessive demand on the computational resources. On the contrary, using a fully unstructured anisotropic mesh results in poorly shaped elements (e.g., those with aspect ratio above 1,000) and leads to a poor numerical approximation of the boundary layer behavior. To remedy these issues, meshes with layered and graded elements near the viscous walls are employed. For complex geometries such meshes are typically composed of triangular elements on the viscous walls that are inflated or extruded into the volume along the wall-normal direction up to a specified height while the rest of the domain is filled with unstructured tetrahedral elements. This type of mesh is referred to as a boundary layer mesh. Usually, linear elements with C0 inter-element continuity are employed and in some situations higher order C0 elements are also used. However, these elements only enforce continuity whereas high-order smoothness is not attained (i.e., C1 inter-element continuity or higher is not attained). High-order analysis on boundary layer meshes must exploit and maintain highly anisotropic, graded and layered elements near the walls. To achieve greater inter-element continuity in a local fashion, we employ B-spline basis functions in the wall-normal direction only in the layered portion of the mesh. This type of basis setting is possible by exploiting the structure of the element stacks in the layered portion of the mesh. For example, Guarini et al. [1] have used B-splines in the wall-normal direction (throughout the domain height) and a spectral basis in the wall-parallel or lateral directions to perform direct numerical simulation of turbulent boundary layer flow over a plate. However, a combination of B-splines and a spectral basis is not applicable to more complex geometries. For more complex geometries, we make use of triangular surface elements in the lateral directions while B-splines are used in the wall-normal direction. This results in basis functions with mixed order as well as mixed continuity. We employ this high-order basis setting within the stabilized finite element analysis (based on variational multiscale method) and demonstrate their effectiveness for boundary layer flow problems including those with a manufactured boundary layer behavior. References: [1] S.E. Guarini, R.D. Moser, K. Shariff and A. Wray, "Direct numerical simulation of a supersonic turbulent boundary layer at Mach 2.5", *Journal of Fluid Mechanics* 414:1-33, 2000.

Title: 1D, 2D, and 3D Unstructured-Grid Modeling of Sediment Transport in a Salt-Marsh Estuary

Author(s): Yun Zhang, Oliver Fringer, *Stanford U.*

We apply the finite-volume, unstructured-grid SUNTANS model to simulate sediment transport in the presence of tides and inflows in a salt marsh estuary in San Francisco Bay. The estuary is characterized by broad, shallow, and densely vegetated marshes that are incised by narrow channels, some of which are engineered to restrict seaward sediment transport with culverts. Owing to the channelized nature of the system and the desire to study sediment transport patterns over seasonal and decadal time scales, we develop a framework that allows the SUNTANS model to simulate the network of channels using a single along-channel dimension. Implementation of subgrid bathymetry ensures that the one-dimensional model captures the same flow rate and stage as the two- and three-dimensional implementations of SUNTANS. We will discuss tradeoffs between accuracy and efficiency of the hierarchy of models, and we will also discuss implementation of a culvert and the marsh drag model and their effects on sediment transport.

Title: Coupled Atomistic-Continuum Framework of Developing Constitutive Relations of Crack Propagation

Author(s): Jiayi Zhang, Subhendu Chakraborty, Somnath Ghosh, *Johns Hopkins U.*

Modeling ductile crack propagation in crystalline materials is a challenging enterprise due to complexities induced by the interaction of crack and plasticity. Atomistic simulation tools have been proven to be powerful in investigating various mechanisms in plastic deformation and crack propagation. However the computational cost puts strong limitation to both spatial and temporal scale of atomistic studies. This could lead to inaccurate results. For example, unrealistic boundary condition on atomistic domain can cause incorrect stress distribution. Moreover, most atomistic studies on dislocation limited on nucleation process since the plastic behavior governed by collective motion of many dislocations cannot be captured within limited domain size. Many efforts have been made to develop and utilize coupled atomistic-continuum methods to overcome the computational limitation of MD simulations, a representative review of many developed methods is given by Tadmor and Miller. In this work, we represent a methodology to investigate crack propagation and cohesive relation using parallel coupled atomistic-continuum methods inspired by early work by Saether etc. The target is to extract the cohesive-type constitutive behavior of crack from the developed coupled model, so that it can be implemented in higher scale finite element analysis. We propose a consistency condition that constitutive relation should obey, i.e. the the extracted continuum model having same energy release rate compared with the result from coupled atomistic-continuum model. Under this framework, we further investigate the length scale effect and gradient effect of the crack constitutive relation. The on-going work includes: extending the analysis into plastic regime by implementing crystal plasticity into continuum domain in the coupled model, and also using hyperdynamics approach to more accurately capture the thermally activated processes.

Title: Heat Conduction in Atomistic/Continuum System Based on Coarse-Grained Molecular Dynamics

Author(s): Zhen Zhang, Jiaoyan Li, James Lee, *George Washington U.*

Coarse-grained molecular dynamics (CG-MD) is a multiscale method for concurrently coupling atomic region and atom-based continuum (ABC) region in a nano/micro material system. In molecular dynamics (MD), temperature is a velocity-dependent quantity and Nosé-Hoover thermostat is often used to gently regulate the local temperature. In CGMD, the temperature of the ABC region does not follow the same equation as in MD because of the significant reduction in the degrees of freedom. We present a simple method for calculating local temperature for ABC region. Based on the ideas of Nosé-Hoover thermostat and the representativeness of nodes in the ABC region, we propose a temperature equation which only requires information of nodes, such as nodal velocities and nodal mass. Besides, an algorithm analogous to Nosé-Hoover thermostat is designed for the ABC region. Therefore, the temperature is obtainable not only in a coupled atom/continuum system, but also in a pure coarse-grained system. We utilize our method to study the heat conduction problem of a MgO specimen. The specimen is divided into two regions. One region is controlled at a constant temperature, while the other region is free from temperature control. The controlled region can be either atomic region or ABC region. The simulation results show that the system is capable of reaching thermal equilibrium, namely the thermal energy successfully transfers from the controlled region to the free region.

Title: A Representative-Sandwich Model for Mechanical-Crush and Short-Circuit Simulation of Lithium-Ion Battery

Author(s): Chao Zhang, Shriram Santhanagopalan, Michael Sprague, Ahmad Pesaran, *Nat'l. Renewable Energy Lab.*

Lithium-ion batteries are currently the state-of-the-art power sources for a variety of applications, from consumer electronic devices to electric-drive vehicles (EDVs). Being an energized component, failure of the battery is an essential concern, which can result in rupture, smoke, fire, or venting [1]. The failure of Lithium-ion batteries can be due to a number of external abusive conditions (impact/crush, overcharge, thermal ramp, etc.) or internal conditions (internal short circuits, excessive heating due to resistance build-up, etc.), of which the mechanical-abuse-induced short circuit is a very practical problem [2]. In order to better understand the behavior of Lithium-ion batteries under mechanical abuse, a coupled modeling methodology encompassing the mechanical, thermal and electrical response has been developed for predicting short circuit under external crush. The combined mechanical-electric-thermal response is simulated in LS-DYNA using a single representative-sandwich (RS) finite-element model based on a sequential analysis, where electrical-thermal modeling is conducted after an instantaneous mechanical crush. The model includes an explicit representation of each individual component such as the active material, current collector, separator, etc., and predicts their mechanical deformation under quasi-static compression and indentation. The single RS models (consist of 8 layers) display significantly better computational efficiency while maintain good accuracy. The numerical results show good agreement with full pouch cell models (explicitly simulate all 163 layers of the battery cell) and experiments. The fracture of the battery structure under different indentation conditions are simulated and studied. On the other hand, the electrical-thermal simulation predicts the current density and temperature distribution in a reasonable manner. We use the electrical contact between active materials following the failure of the separator as a criterion for short circuit. The evolution of electrical properties and initiation of short circuit during the mechanical crush are well predicted. The modeling technique is useful in studying the safety behavior of Lithium-ion cells under mechanical abuse and can be helpful in the design of more efficient and safer battery structures. References: [1] Lu, Languang, et al. "A review on the key issues for lithium-ion battery management in electric vehicles." *Journal of power sources* 226 (2013): 272-288. [2] Sahraei, Elham, Rich Hill, and Tomasz Wierzbicki. "Calibration and finite element simulation of pouch lithium-ion batteries for mechanical integrity." *Journal of Power Sources* 201 (2012): 307-321.

Title: Peridynamic Modeling of Dynamic Brittle Failure in Polycrystalline Ceramics

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

A peridynamic (PD) model is proposed to simulate dynamic brittle fracture in polycrystalline materials with cubic symmetry. As a particular example, we model failure evolution from edge-on impact in AION. Since elastic wave propagation and wave reinforcements are the main causes of damage initiation and growth in dynamic brittle fracture, parameters in this model are determined by matching longitudinal wave speed along different propagation directions ([100], [110], and [111]) of a single crystal sample. Micromodulus of peridynamic bonds is evaluated in the grain coordinate system that is correlated with the sample coordinate by a transformation matrix. Because, in general, grain boundaries are softer than the grains, for the peridynamic bonds that connect two different grains, we select their micromodulus as the smaller of the two corresponding stiffnesses associated with the two orientations of the bond in the two corresponding grains. In the present model, we use a critical bond elongation that does not depend on the orientation or on the location of the nodes at the end of the bond. This choice is motivated by the experimental evidence that shows mixed transgranular and intergranular fracture in AION from impact. Some transgranular fracture surfaces observed in AION fragments are similar to conchoidal cracks in homogeneous materials. In the future, to be able to model materials with clearly defined cleavage planes, like sapphire, we will use critical bond elongations that strongly depend on the orientation of the bond. We simulate a polycrystalline AION sample of millimeter dimensions (with about 200 grains generated by Voronoi tessellation) under edge-on impact conditions to investigate the mechanisms of dynamic fracture. In the peridynamic model, we use a nonlocal region (the PD horizon) that is 1/10 of the average grain size. This is small enough to simulate the influence of microstructure on failure front and fracture propagation. Simulation results match experimental results very well. The PD results include intergranular and transgranular fracture. The surface of the sample shows a coherent damage zone moving through the material at relatively high speed. When the failure front stops from advancing, damage transitions to individual, localized cracks that initiate from the edge of the failure front and move at a much lower propagation speeds than the failure front. Both the failure mechanisms and the propagation speeds are well captured by our PD model.

Title: Reduced-Basis Method for Variational Inequalities in Contact Mechanics

Author(s): Zhenying Zhang, *AICES, RWTH Aachen*; Karen Veroy, *AICES, RWTH Aachen*.

We present an efficient model order reduction method [1] for parametrized elliptic variational inequalities of the first kind: find u in an admissible convex set K composed by an inequality constraint, such that it minimizes the energy function. Motivated by numerous engineering applications that involve contact between elastic body and rigid obstacle, e.g. the obstacle problem [2], we develop a primal-dual reduced basis approach to construct offline-online efficient yet certified reduced order models. Such models find application in the real-time or many query context of PDE-constrained optimization, control, or parameter estimation. They can also be easily extended to parabolic systems [3]. Firstly, we develop a primal-dual certified reduced basis method for bijective constraint operator B that provides sharp and inexpensive a posteriori error bounds. We compare both the proposed error bounds and the computational costs with the proposed method in [4], demonstrating the quality and effectivity of the approximation and the error bounds. Then, we extend our results to more generalized problems, namely a surjective constraint operator B as appears, e.g. in Signorini's Problem. We present both a priori and a posteriori analysis for the generalized formulation [2] and the saddle point formulation [5]. Lastly, we discuss the construction and sampling procedure [1] for the given method. References [1] A. T. Patera, G. Rozza. Reduced Basis Approximation and A Posteriori Error Estimation for Parametrized Partial Differential Equations. Version 1.0, Copyright MIT 2006, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering. [2] R. Glowinski. Numerical Methods for Nonlinear Variational Inequalities. Springer, 2008. [3] M. A. Grepl, A. T. Patera. A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations. ESAIM: Math. [4] B. Haasdonk, J. Salomon, and B. Wohlmuth. A reduced basis method for parametrized variational inequalities. SIAM J. Numer. Anal. 2012. [5] F. Brezzi, M. Fortin. Mixed and Hybrid Finite Element Methods. Springer-Verlag, 1991.

Title: A Discrete Filter Scheme for Large-Scale Topology Design of 3D Structures Using the Ground Structure Method

Author(s): Xiaojia Zhang, Glaucio Paulino, *Georgia Inst. Tech.*; Adeildo Ramos Jr, *Federal U. Alagoas* .

Topology optimization of trusses, using the ground structure method, is a practical tool that allows for improved designs with minimal design iterations. However, the final topology consists of a considerable number of undesirable thin bars, the removal of which can result in a violation of global equilibrium. Therefore, although the solution by the optimization process is optimal in some sense, manufacturing may be infeasible. To address this issue, we propose an efficient discrete filter scheme that applies to large scale two- and three-dimensional topology optimization of trusses using the ground structure method. This technique produces well-defined three-dimensional structures that allow for direct manufacturing and practical design. Because the final layout is user-adjustable and consists of a finite number of bars, it is conducive to additive manufacturing. Furthermore, we show that the final topology satisfies global equilibrium and demonstrate the efficiency of the proposed technique in large-scale topology optimization problems. For demonstration purposes, we present several practical design problems and illustrate the applications of each problem addressed.

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Title: Truncated Hierarchical Catmull-Clark Subdivision with Local Refinement

Author(s): Xiaodong Wei, Yongjie Zhang, *Carnegie Mellon U.*; Thomas Hughes, *UT Austin*; Michael Scott, *Brigham Young U.*

In this talk, we present a new method termed Truncated Hierarchical Catmull-Clark Subdivision (THCCS), which generalizes truncated hierarchical B-splines to control grids of arbitrary topology. THCCS basis functions satisfy partition of unity, are linearly independent, and are locally refinable. THCCS also preserves geometry during adaptive h-refinement and thus inherits the surface continuity of Catmull-Clark subdivision, namely C2-continuous everywhere except at the local region surrounding extraordinary nodes, where the surface continuity is C1. Recently, we also develop a basis-function-insertion scheme with the aid of truncation mechanism, which refines one-ring neighboring elements rather than two-ring in the original development of THCCS. The new scheme significantly improves the efficiency of local refinement. Adaptive isogeometric analysis is performed with THCCS basis functions on a benchmark problem with extraordinary nodes. Local refinement on complex surfaces is also studied to show potential wide application of the proposed method.

Title: Modified Peridynamic Model and Its Application in Penetration Problem of Concrete Slabs

Author(s): Qing Zhang, Xin Gu, Dan Huang, *Hohai U.*

Peridynamics uses uniform spatial-integral and time-differential equations to describe continuous or discontinuous deformation characteristics of materials and structures. It has been utilized successfully in the past decades for the analysis of fracture problems at both macro- and micro-scales, especially in cracking problem and impact problem. Constructing a constitutive force function is paramount in peridynamic modeling, and the widely used pairwise constitutive force function in PMB model has a constant micromodulus, which cannot indicate the size effect of long range force and affect the numerical accuracy. We think that the long range constitutive force should meet three features: diminishing value with increasing distance, finite value and following Newton's Third Law. In this paper, the micromodulus of the pair-wise bond, which is described as a continuous function of the distance between two particles within the material horizon, and which is demonstrated to be more accurate compared to the previous PD models using a fixed stiffness constant to describe the interaction of particles. To study the failure process, the final failure patterns and its mechanism of concrete under impact loading are extremely important in civil and military engineering. An impact contact algorithm to describe interaction between rigid projectile and deformable target body is proposed, and the explicit dynamic method to solve the peridynamic equations is used in the present paper. The capability of the modified bond-based peridynamic model in analyzing impact problem is validated through the well-known Kalthoff-Winkler experiment. Furthermore, some 3D concrete slabs subjected to rigid sphere projectile impact with different velocities are simulated. The simulation results reveal explicitly the final failure patterns, the accumulated damage and the progressive failure process of concrete slabs, which have significant differences under different velocities. Numerical simulations illustrate that the modified peridynamic model is reasonable and reliable, and peridynamics is an effective method in simulating the impact problems of concrete structures. Reference: [1] Silling S.A. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 2000, 48: 175-209. [2] Demmie P, Silling S. An approach to modeling extreme loading of structures using peridynamics[J]. *Journal of Mechanics of Materials and Structures*, 2007, 2(10): 1921-1945. [3] Huang D, Zhang Q, Qiao P Z. Damage and progressive failure of concrete structures using non-local peridynamic modeling[J]. *Science China Technological Sciences*, 2011, 54(3): 591-596.

Title: An Explicit Formula for the Coherent SH Waves' Attenuation Coefficient in Random Porous Materials with Low Porosities

Author(s): Jun Zhang, *Chongqing U.*; Wenjing Ye, *Hong Kong U. Sci. Tech.*.

In this work, the attenuation coefficient of coherent SH waves in random porous material with uniform randomly distributed elliptical cavities of different aspect ratios is studied. Based on the analysis of the mechanism for attenuation, a simple macro model for the attenuation coefficient is proposed. The macro model says that the attenuation coefficient can be expressed as a function of the mean scattering cross section and the number density of cavities at low porosities. Then, large-scale numerical simulations using the pre-corrected Fast Fourier Transform (pFFT) algorithm accelerated Boundary Element Method are conducted to specify this macro model. Finally, this macro model is compared with four theoretical models derived for composite/porous materials with circular inclusions at the porosity $p=3.17\%$ and 5% . Results show this macro model agree well with three of them. Compared to the existing relevant works, the form of this macro model is simple and has a clear physical meaning. In addition, it is applicable to cases with relatively complex cavities.

Title: A Dynamically Bi-Orthogonal Method for Time-Dependent Stochastic Partial Differential Equation

Author(s): Mulin Cheng, Thomas Hou, Zhiwen Zhang, *Caltech*.

We propose a dynamically bi-orthogonal method (DyBO) to study time dependent stochastic partial differential equations (SPDEs). The objective of our method is to exploit some intrinsic sparse structure in the stochastic solution by constructing the sparsest representation of the stochastic solution via a bi-orthogonal basis. It is well-known that the Karhunen-Loeve expansion minimizes the total mean squared error and gives the sparsest representation of stochastic solutions. However, the computation of the KL expansion could be quite expensive since we need to form a covariance matrix and solve a large-scale eigenvalue problem. In this talk, we derive an equivalent system that governs the evolution of the spatial and stochastic basis in the KL expansion. Unlike other reduced model methods, our method constructs the reduced basis on-the-fly without the need to form the covariance matrix or to compute its eigen-decomposition. We further present an adaptive strategy to dynamically remove or add modes, perform a detailed complexity analysis, and discuss various generalizations of this approach. Several numerical experiments will be provided to demonstrate the effectiveness of the DyBO method.

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Title: Quasi-Optimal Approximations of Parameterized PDEs with Deterministic and Stochastic Coefficients

Author(s): Clayton Webster, Hoang Tran, Guannan Zhang, *ORNL*; Ron DeVore, *Texas A&M U.*

In this talk, we present a generalized methodology for analyzing the convergence of quasi-optimal polynomial and interpolation approximations, applicable to a wide class of parameterized PDEs with both deterministic and stochastic inputs. Such quasi-optimal methods construct an index set that corresponds to the “best M-terms,” based on sharp estimates of the polynomial coefficients. In particular, we consider several cases of N dimensional affine and non-affine coefficients, and prove analytic dependence of the PDE solution map in a polydisc or polyellipse of the multi-dimensional complex plane respectively. The framework we propose for analyzing asymptotic truncation errors of quasi-optimal methods is based on an extension of the underlying multi-index set into a continuous domain, and then an approximation of the cardinality (number of integer multi-indices) by its Lebesgue measure. Several types of isotropic and anisotropic (weighted) multi-index sets are explored, and rigorous proofs reveal sharp asymptotic error estimates in which we achieve sub-exponential convergence rates with respect to the total number of degrees of freedom. Through several theoretical examples, we explicitly derive the rate constant and use the resulting sharp bounds to illustrate the effectiveness of our approach, as well as compare our rates of convergence with current published results. Finally, computational evidence complements the theory and shows the advantage of our generalized methodology compared to previously developed estimates.

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Title: Quasi-Optimal Approximations of Parameterized PDEs with Deterministic and Stochastic Coefficients

Author(s): Guannan Zhang, Hoang Tran, Clayton Webster, *Oak Ridge Nat'l. Lab.*

In this talk, we present a generalized methodology for analyzing the convergence of quasi-optimal polynomial and interpolation approximations, applicable to a wide class of parameterized PDEs with both deterministic and stochastic inputs. Such quasi-optimal methods construct an index set that corresponds to the “best M-terms,” based on sharp estimates of the polynomial coefficients. In particular, we consider several cases of N dimensional affine and non-affine coefficients, and prove analytic dependence of the PDE solution map in a polydisc or polyellipse of the multi-dimensional complex plane respectively. The framework we propose for analyzing asymptotic truncation errors of quasi-optimal methods is based on an extension of the underlying multi-index set into a continuous domain, and then an approximation of the cardinality (number of integer multi-indices) by its Lebesgue measure. Several types of isotropic and anisotropic (weighted) multi-index sets are explored, and rigorous proofs reveal sharp asymptotic error estimates in which we achieve sub-exponential convergence rates with respect to the total number of degrees of freedom. Through several theoretical examples, we explicitly derive the rate constant and use the resulting sharp bounds to illustrate the effectiveness of our approach, as well as compare our rates of convergence with current published results. Finally, computational evidence complements the theory and shows the advantage of our generalized methodology compared to previously developed estimates.

Title: Constitutive Modeling for Additive Manufactured Photopolymers Considering the Effect of Print Orientation

Author(s): Pu Zhang, Albert To, *U. Pittsburgh.*

Photopolymerization is one of the dominating and well-developed techniques used in additive manufacturing (AM) technology. Its high resolution and precision are unbeatable compared with other AM processes for polymers. Therefore, it is of great significance to investigate and model the mechanical performance of the AM photopolymers for engineering component design and analysis. Our experimental test indicates that the AM photopolymers (e.g. VeroWhitePlus) show strong printing orientation effect on mechanical properties of the printed material. The elastic response of the AM photopolymer is transversely isotropic with the privileged axis along the printing direction. In addition, the photopolymer behaves like a brittle material along the printing direction, while its in-plane post-yielding response is rather ductile. Hence, a transversely isotropic hyperelastic-viscoplastic constitutive model is proposed to predict the nonlinear and anisotropic behaviors of AM photopolymers. In addition, the Tsai-Wu failure criterion is adopted to predict the anisotropic failure behavior. Experimental tests are conducted on tensile and compressive photopolymer specimens manufactured along different printing orientations. The proposed constitutive model and failure criterion are fitted from the experimental data.

Title: Numerical Noises in Various Material Point Methods

Author(s): Duan Zhang, *Los Alamos Nat'l. Lab.*

One of the significant advantages of the particle methods is their capability of tracking material deformation history in a large material deformation. It is now well known that the original material point method (MPM) suffers from numerical noises due to particles moving across cell boundaries in cases of large material deformation. To overcome this numerical difficulty, three improved MPM versions have been developed. They are the generalized interpolation material point (GIMP) method, the convected particle domain interpolation (CPDI) method, and the dual domain material point (DDMP) method. Since many large material deformation problems involve propagation of shocks, before applying these particle methods to more complicated problems, we examine their numerical properties in a very simple problem – shock wave propagation in an ideal gas. To our surprise, we find that MPM cannot be used. The GIMP, CPDI and DDMP methods are usable. For a strong shock, all the three methods produce reasonable solutions. In general, numerical properties of GIMP and CPDI are quite similar. Contrary to our intuition, weak shocks are more challenging for the particle methods. GIMP and CPDI performs better than DDMP in calculations with low spatial resolutions (large cells and small number of particles per cell), however they do not show significant trend of convergence as mesh and particle size are refined. The DDMP method shows correctly convergence trend, but fine resolutions are required to obtain satisfactory results. To improve performance of DDMP method at low spatial resolutions, we introduce a new integration scheme using daughter particles. The new integration scheme results in significant improvements of the numerical results.

Title: Element-Free Analysis of Some Mathematical Problems

Author(s): L.W. Zhang, *City U. Hong Kong* ; K.M. Liew, *City U. Hong Kong*.

An element-free framework based on the improved moving least-squares Ritz (IMLS-Ritz) method is employed for solving some mathematical problems [1]. Employing the IMLS approximation for the field variables, discretized governing equations of the problems are derived via the Ritz procedure. Using the IMLS approximation, an orthogonal functional system having a weight function is used to construct the displacement fields. The resulting algebraic equation system can be solved without a matrix inversion. As a result of the above procedures, the final algebraic equation system is derived through discretizing the constructed energy functional. The functional is established by enforcing the Dirichlet boundary conditions via the penalty approach. Convergence studies are carried out to examine the numerical stability of the IMLS-Ritz method by considering the influences of support sizes, number of nodes and time steps involved [2, 3]. The accuracy of the method can be enhanced by increasing number of terms used in the shape functions. A few numerical examples are selected, i.e. the one-dimensional nonlinear Klein-Gordon equation, two-dimensional spatial diffusion of biological population problem, and three-dimensional wave equation. These problems are used to illustrate the simplicity and accuracy of the numerical solution method. The accuracy is validated by comparing the IMLS-Ritz results with the analytical solutions. From this study, it is concluded that the IMLS-Ritz method may be readily applied to find numerical solutions for a wide range of PDEs in the fields of mathematics and engineering. [1] L.W. Zhang, K.M. Liew. An improved moving least-squares Ritz method for two-dimensional elasticity problems, *Applied Mathematics and Computation*, 246 (2014) 268-282. [2] L.W. Zhang, Y.J. Deng, K.M. Liew. An improved element-free Galerkin method for numerical modeling of the biological population problems, *Engineering Analysis with Boundary Elements*, 40 (2014) 181-188. [3] L.W. Zhang, Y.J. Deng, K.M. Liew, Y.M. Cheng. The improved complex variable element-free Galerkin method for two-dimensional Schrödinger equation, *Computers and Mathematics with Applications*, 68 (2014) 1093-1116.

13th U.S. National Congress on Computational Mechanics
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Title: Accelerated Simulation of Structural/Material Dynamics Based on Space-Time, Finite-Element Method

Author(s): Rui Zhang, *Northwestern Polytech. U.; UT Dallas*; Lihua Wen, *Northwestern Polytech. U.*; Dong Qian, *UT Dallas*.

In developing computational approaches for mechanical responses with a wide range of spatial and temporal scales, space-time finite element is emerging as an interesting method as it provides an entire different way of treating the temporal scales when compared with the traditional FEM based on semi-discrete schemes. With this unique feature, past study has shown that space-time formulations such as these based on the discontinuous Galerkin approach significantly reduces the artificial oscillations that are commonly associated with semi-discrete time integration schemes in capturing sharp gradients. In addition, this class of methods has been shown to be both higher order accurate and unconditionally stable. While the robustness of the space-time method has been extensively demonstrated, a critical barrier for the extensive application is the large computational cost associated with the additional time dimension that is introduced. As such, the extended capability of the method is paid at the price of converting an n -dimensional spatial problem to an $n+1$ dimensional problem, which, if not properly treated, can lead to prohibitive computational expense. The main objective of this talk is to explore techniques that can be employed to accelerate the computation of both the space-time FEM and the enriched version that was recently developed [1, 2]. It is shown that drastic reduction in the computing time can be accomplished through a general approach. With the proper preconditioning, the computational cost scales with the number of degree of freedom through $\sim O(N^{1.5})$. Finally, we demonstrate the accelerated space-time FEM simulation through extensive benchmark problems. [1] S. Bhamare, T. Eason, S. Spottswood, S. Mannava, V. Vasudevan, and D. Qian, "A multi-temporal scale approach to high cycle fatigue simulation," *Computational Mechanics*, pp. 1-14, 2013/08/29 2013. [2] S. U. Chirputkar and D. Qian, "Coupled atomistic/continuum simulation based on extended space-time finite element method," *Cmes-Computer Modeling In Engineering & Sciences*, vol. 24, pp. 185-202, Feb 2008.

Title: Computational Equilibria of Two-Phase Lipid Bilayer Vesicles via Global Symmetry-Breaking Bifurcation

Author(s): Siming Zhao, Timothy Healey, *Cornell U.*

In this work, we use Helfrich-Cahn-Hilliard phase field model to study the phase transition and deformation behavior of two-phase lipid bilayer vesicles, using global symmetry-breaking bifurcation methods. The well-known difficulty associated with the in-plane fluidity of lipid membranes is removed by employing a radially projected coordinate system from the perfect spherical state. This enables the direct computation of shape change without requiring knowledge of the completely underdetermined in-plane fluid displacements. The sub-division surface finite element [1] is employed to construct our discrete model, which achieves the necessary C1 continuity with just one degree of freedom per node. Standard bifurcation theory cannot be directly applied due to the high dimensional null spaces of the linearization – a direct consequence of $O(3)$ symmetry. We employ well known group-theoretic projection techniques [2] to accurately compute solution branches having prescribed symmetries – corresponding to specific subgroups of $O(3)$. In particular, the icosahedral subgroup is chosen here to capture the “soccer-ball” shapes observed in experiments [3]. Through numerical continuation in multi-parameters, we are able to systematically explore the model’s rich phase transition and deformation behavior. In particular, we pinpoint the aforementioned soccer balls and determine their stability. [1] Cirak, F., Ortiz M., and Schroder P. "Subdivision surfaces: a new paradigm for thin-shell finite-element analysis." *International Journal for Numerical Methods in Engineering* 47.12 (2000): 2039-2072. [2] Healey, T.J. "A group-theoretic approach to computational bifurcation problems with symmetry." *Computer Methods in Applied Mechanics and Engineering* 67.3 (1988): 257-295. [3] Baumgart, T., Samuel T. H., and Watt W.W. "Imaging coexisting fluid domains in biomembrane models coupling curvature and line tension." *Nature* 425.6960 (2003): 821-824.

Title: Modelling of Fabric Composite Mesoscale Response Under Hypervelocity Impact

Author(s): Shicao Zhao, *Inst. Computer App. CAEP.*

High performance fiber fabric composites are widely used in spacecraft protective structures. To resist hypervelocity impact (HVI) of space debris or meteorites with an average velocity up to 10 km/s, the fabrics are usually filled into the normal whipple structure, which is made up of an aluminum alloy metal bumper and the backwall to be protected. During a debris impact progress, the bumper and the impacted debris are broken into fragments called debris cloud which will expand in the space between bumper and backwall. Due to the high modulus, micrometer size and brittle failure characteristics of high performance fiber such as SiC or Carbon Fiber, the fragments size turned to be much smaller when debris cloud impacts the filled fabrics to ensure the debris cloud expand more widely and well-distributed. Due to the extremely high impact speed in the space, the shock wave theory must be considered. Different from many mesoscale method of Composite Mechanics, composite under hypervelocity impact will undergo the phase change. The phase diagram of fiber and matrix can be such different that matrix will be lose their solid status in serval microseconds after impact. This kind of phenomenon can be found in our experiment results clearly. In this situation, the shock response of fabrics is nonhomogeneous in nature, and strong localization prevails in such a short duration of several microseconds, then a discretization numerical method will be suitable, especially when the object of study is debris cloud. So we use the mesh-free SPH method to build the fiber and matrix respectively due to the mismatch of modulus and strength between them, which will definitely effect shock wave structure. To consider the meso-structure of fabric, the fiber itself is to be modeled as the real texture to describe the different failure mode and fragment size distribution. Different from the homogeneous continuum model, the material parameters, such as elastic modulus and strength are determined from the properties of fibers and matrix materials. The global feature of anisotropy is therefore implicit in the fabric texture of the composite.

Title: On the Ground Structure Method Accounting for Buckling and Nodal Instability

Author(s): Tuo Zhao, Glaucio Paulino, *Georgia Inst. Tech.*.

The typical layout optimization problem with plastic formulation consists of minimizing the total volume of material while satisfying nodal equilibrium constraint and predefined stress limits. Here we consider the ground structure approach. However, such an approach may lead to very slender members and unstable nodes that might cause instability issues. To address this issue, we implement the plastic formulation using constraints that account for instability i.e. buckling and nodal instability either together or in isolation. We use as constraints in the implementation the Euler buckling criteria and the nominal lateral force while also addressing the efficiency of the nonlinear programming. To illustrate the features of the implementation, we present numerical examples in both 2D and 3D structures, the latter accounting for more realistic structures. We obtain convergent results which lead to more stable structures. Those final optimum structures as well as the initial latticed ground structures are prototyped via Selective Laser Sintering as the additive manufacturing technology of choice. Such a prototyping can assist engineers in the early conceptual design phase in e.g. architecture and industrial design engineering. Those prototypes can also be used as educational tools for teaching structural optimization in a classroom environment.

Title: A Strong Coupling Phase Field Model Accounting for the Effect of Plastic Deformation Energy on Grain Growth

Author(s): Lei Zhao, Izabela Szlufarska, *U. Wisconsin*; Pritam Chakraborty, Michael Tonks, *Idaho Nat'l. Lab.*

During large plastic deformation of metals, the stored plastic deformation energy is significant compared to other free energy contributions, and therefore plays an important role in driving the microstructural evolution. We developed the first integrated grain growth model that concurrently couples phase field method with crystal plasticity finite element analysis to study the microstructural evolution of copper polycrystals subjected to large deformation. In particular, we implement a stress interpolation scheme to extend single-crystal constitutive equations to calculations of stress components on grain boundaries. The stored plastic deformation energy is expressed in the form of a latent hardening term, which in turn is based on a non-convex plastic potential model proposed by Ortiz and Repetto [1]. First, we derived the plastic potential driving force with no direct dependence on dislocation density and we coupled this driving force into Ginzburg-Landau equation to study the effect of plastic behavior on grain boundary network evolution. Then, the derived plastic potential driving force was validated against an analytical expression for plastic driving force, which analytical expression depends on dislocation energy [2]. A bicrystal simulation is used to demonstrate the validity of our integrated model. In this presentation, we will also discuss similarities and differences in the effects of plastic behavior on grain growth as predicted by our newly developed strong coupling model and a weak coupling model. Our developments provide a useful tool for simulating microstructural evolution in metals undergoing large plastic deformations, e.g., during cold- and hot-working and during frictional sliding. All these developments have been implemented in the MOOSE/MARMOT simulation package. [1] Michael Ortiz and EA Repetto. Nonconvex energy minimization and dislocation structures in ductile single crystals. *Journal of the Mechanics and Physics of Solids*, 47(2):397–462, 1999. [2] Gunter Gottstein and Lasar S Shvindlerman. Grain boundary migration in metals: thermodynamics, kinetics, applications. CRC press, 1999.

Title: Identification of Key Microstructure Features in the Design of Nanocomposites

Author(s): RAMIN BOSTANABAD, Anqi Hu, Wei Chen, L. Catherine Brinson, He Zhao, *Northwestern U.*

Considerable research is done on computational material design to reduce the costly and time-consuming reliance on experimental approaches. These efforts are hindered by (1) the high dimensional microstructure design space (2) the cumbersome procedure for material reconstruction corresponding to a design point and (3) the expensive search for finding the optimum design. In this work, we propose a three-phase approach for the fast and efficient design of polymer nanocomposites to obtain optimum material properties. In the first phase, the high dimensional design space is represented with a finite set of physical descriptors that embrace various morphological features (of each constituent) such as volume fraction, spatial distribution, and geometry of the inclusions. Next, Design of Experiments (DOE) is used to efficiently explore the new design space. In particular, constrained optimum Latin Hyper Cube is utilized to satisfy the constraints associated with the range of the descriptors while optimally exploring the design space. In phase two, a hierarchical reconstruction algorithm is used to efficiently generate the microstructures corresponding to each sample design point. The hierarchical nature of the algorithm decouples fine and coarse reconstructions and makes the process parallelizable. Afterwards, the properties of interest of polymer nanocomposites are calculated via Finite Element Analysis (FEA). In the last phase, state-of-the-art metamodeling techniques are used to establish a mapping between the physical descriptors (design inputs) and evaluated properties (responses). Specifically, Kriging model is chosen over other methods due to its capabilities in quantifying the uncertainty within the whole design space as well as its flexibility in fitting nonlinear functions. This process is followed by statistical sensitivity analysis to determine the key physical descriptors affecting the material properties and to reduce the dimensionality of the problem if necessary. The constructed structure-property relations at the nanoscale can be used to explore the optimal design of filler morphology and further integrated into meso-scale representative volume element models to predict the bulk properties of nanocomposite systems.

Title: A Phase-Field Method for Simulation of Two-Phase Flow Induced Pipe Vibration

Author(s): Xiaoning Zheng, *MIT*; George Karniadakis, *Brown U.*

We present a phase-field method for simulating two-phase flow induced vibration of a pipe. To this end, we solve the Navier–Stokes equations, Cahn-Hilliard equation and structural equation in an arbitrary Lagrangian Eulerian (ALE) framework. A spectral/hp element method is employed for spatial discretization and backward differentiation formulae (BDF) is employed for time discretization. Simulation results about annular two-phase internal flow induced vibration of a pipe are compared with theoretical and experimental data in literature. Using this phase-field method, we investigate the effect of two-phase flow characteristics upon the natural frequencies of vibration of a pipe. Both internal and external flow with respect to a pipe are considered.

Title: Dynamic Instability of Slender Curved Structures

Author(s): Yang Zhou, Ilinca Stanciulescu, *Rice U.*

Slender curved structures (e.g., shallow arches and curved panels), commonly used in the civil, mechanical and aerospace engineering, have high risk of losing stability well before the strength limit is reached. One type of instability that a curved structure frequently exhibits is snap-through, where the structure suddenly jumps from its initial configuration to a remote coexisting equilibrium configuration with reverse curvature. When a curved structure with such underlying static behavior is subjected to dynamic load, it can exhibit dynamic snap-through with large amplitude oscillations between remote coexisting equilibrium states. The persistent dynamic snap between remote configurations results in frequent large stress reversals and greatly exacerbates the fatigue failure. In the design and optimization of a curved structure under dynamic load, it is of great importance to identify the dynamic stability boundary that separates the small amplitude non-snap and the large amplitude post-snap oscillations in the space of the forcing amplitudes and frequencies. Since the analytical solutions for such highly nonlinear phenomena are typically not available, a parametric numerical study with thousands separate transient simulations is usually required to obtain one such dynamic stability boundary. If a parameter such as the geometry of the structure changes, which occurs very often in the design and optimization process, the transient simulations need to be performed for the new condition. The total computational cost to obtain the dynamic stability boundaries of many different cases can be very high. To alleviate this high computational cost, we propose techniques to identify the evolution of the dynamic stability boundaries with changes in geometrical parameters defining the structure. Once the dynamic stability boundary for a specific geometry is obtained, the boundaries for other geometries can be quickly estimated without running additional extensive transient simulations.

Title: An Atomistically Validated Continuum Model for Strain Relaxation and Misfit Dislocation Formation

Author(s): Xiaowang Zhou, Donald Ward, Jonathan Zimmerman, Jose Luis Cruz-Campa, James E. Martin, Frank B. Van Swol, *Sandia Nat'l. Labs.*; David Zubia, *UT El Paso*.

A new continuum model of misfit dislocation formation that improves over the traditional model has been developed. This is achieved by developing a robust molecular dynamics (MD) approach that can confidently validate the continuum model. We find that the enabling techniques to make this possible are (a) the calculations of time averaged properties using very long time MD simulations, which produce significantly more accurate results than molecular statics simulations, and (b) the use of dislocation dipole configurations under periodic boundary conditions, which allows dislocation energies to be exactly calculated. Using these techniques, we are able to accurately determine the dislocation core radius and energy without imposing continuum boundary conditions that had to be assumed in previous MD approaches to avoid the effects of truncating long-range dislocation stress fields. The total dislocation energy as a function of system sizes and dislocation spacing predicted from the MD is in very good agreement with the continuum theory. A detailed study reveals that the traditional misfit dislocation model can become inaccurate for systems with large lattice mismatch. We then propose improvements of the theory, including a more accurate treatment of dislocation energies, an incorporation of elastic inhomogeneity from the film and the substrate, and an identification of precise definitions of dislocation spacing and Burgers vector which were likely incorrectly applied in previous work. We show that the prediction from the modified continuum model is essentially indistinguishable from the MD results.

Title: An Experimental and Modeling Investigation on the Shape Evolution of the Cell Nuclei During Closed Mitosis

Author(s): Qian Zhu, Chuanhai Fu, Yuan Lin, *U. Hong Kong.*

Lower eukaryotes, such as the fission yeast (*Schizosaccharomyces pombe*), undergo closed mitosis during which the nuclear envelope (NE) stays intact but changes shape dramatically, usually from a sphere to an ellipsoid and then to a dumbbell for wild-type cells. In comparison, the NE in gene-deletion mutants of the yeast can undergo asymmetric division which often involves tethering or budding of the nuclear membrane. Although it is widely known that closed mitosis is driven by the pushing forces generated among microtubules (MTs), connecting two spindle pole bodies (SPBs) residing at each end of the cell, and associated protein motors, the fundamental question of why and how distinct shape transformations of the NE take place is still poorly understood. Here we report a combined experimental and theoretical study to address this important issue. Specifically, shape evolution of the cell nuclei in the wild-type and different mutants, with known gene defects, of fission yeast was closely monitored with live-cell imaging at high temporal resolution. Interestingly, it was found that structural deficiencies in one or both SPBs will cause the improper assembly and anchoring of mitotic spindle microtubules and ultimately lead to the formation of a single or multiple tethers. On the theoretical side, a physical model was also developed to predict the nuclear shape during mitosis based on energetic considerations. Our model suggests that, in addition to the bending rigidity and surface energy of the nuclear membrane, the spatial distribution of internally generated forces on the NE plays a key role in its shape transformation, with forces localized on both poles of the cell resulting in membrane tethering while a load distribution over a broad area typically leading to the formation of two equal-sized spherical daughter nuclei. These results provide physical explanations on how complex shapes of the nuclear envelope are developed during cell division as well as elucidate their correlations with structural alterations in the nuclear-cytoskeleton, as indicated in our experiments.

Title: Developing XFEM Methodology to Simulate Fracking in Shale

Author(s): Zhuo Zhuang, Zhanli Liu, Dandan Xu, Qinglei Zeng, Tao Wang, *Tsinghua U.*

There are two kernel technologies in extraction shale oil and gas, namely horizontal drilling and hydraulic fracturing, the latter is aka fracking. However, the fracking to result in developing submicron cracks, branching or interactions, and eventually evaluating the crack network still remain enigma. An enhanced extended finite element method (XFEM) is developed to investigate this issue. The fluid pressure as a function of crack geometry is considered in the algorithm. Benchmark problems are carried out to verify the method and program. Crack propagation in shale is divided by different levels, like main crack, submicron crack and crack family. The stability propagation of cracks in different levels is a crucial issue, which may result in a large damage ratio in a represented volume element (RVE). The more damage, the much more permeability is. A large 3D shale physical rock sample with 1.0m³ size experiment of hydraulic fracturing was carried out. The experiment data are compared with numerical solutions.

Title: The Partition of Unity Method as a Coupling Framework

Author(s): Marc Alexander Schweitzer, Sa Wu, *U. Bonn*; Albert Ziegenhagel, *Fraunhofer Inst for Algor. & Sci. Comp.*

Generalized finite element methods obtain their approximation power from the use of problem dependent enrichment functions. This allows for the straightforward inclusion of knowledge obtained from various local or localized methods to obtain a better global solution. In particular, with the means of interpolating scattered data, we may improve our global solution from localized particle methods, or other methods not traditionally associated with (generalized) finite elements. In the context of damage evolution, a discretization of Peridynamics offers an interesting and natural approach to obtain a particle method whose solution covers the damage evolution. In the context of composites, various means of numerical homogenization are known for finite elements and generalized finite elements. We present some findings of using these methods in a localized fashion to obtain enrichments for a Partition of Unity Method from the standpoint of using the PUM as framework for coupling various problem-dependent methods with a Finite Element Method. [1] M.A. Schweitzer, "Generalizations of the finite element method", *Cent. Eur. J. Math.*, 10, 3-24 (2014). [2] M.A. Schweitzer and S. Wu, "Numerical integration of on-the-fly-computed enrichment functions in the PUM", *Meshfree Methods for Partial Differential Equations VII, Lecture Notes in Computational Science and Engineering*, 100, Springer, 2014.

13th U.S. National Congress on Computational Mechanics
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Title: Microstructural Modeling of the Behavior of Crystalline Alloys

Author(s): Qifeng Wu, S. Ziaei, Mohammed Zikry, *North Carolina State U.*

Different aspects of modeling with a specific focus on microstructural characteristics, such as dislocations, precipitates, dispersed particles, grain-boundaries (GBs), and crystallographic slip that span the nano to the micro, and how these characteristics affect failure modes, such as dynamic fracture and hydrogen diffusion assisted fracture. Recently developed fracture methodologies based on overlapping elements have also been used for a detailed analysis of fracture nucleation and the characterization of intergranular and transgranular crack growth. Criteria for dislocation-density interactions and immobilization are directly related to crack blunting and deflection for applications related to martensitic steels and zirconium alloys.

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Title: Atomistic Study of Helium-3 Bubble Growth in Aging Palladium Tritides

Author(s): Jonathan Zimmerman, *Sandia Nat'l. Labs.*; Lucas Hale, *Nat'l. Inst. Stnds. & Tech.*; Bryan Wong, *UC Riverside*.

Palladium is an attractive material for hydrogen-isotope storage applications. One such application is the storage of tritium, but for this application the material's structural and mechanical integrity is threatened by both the embrittlement effect of hydrogen, and the creation and evolution of additional crystal defects (e.g. dislocations, stacking faults) caused by the formation and growth of helium-3 bubbles. Here, we present results that use recently developed inter-atomic potentials for a palladium alloy system within molecular dynamics simulations to examine the defect-mediated mechanisms that govern helium bubble growth. Our simulations show the evolution of a distribution of material defects, and we compare the material behavior displayed with expectations from experiment and theory. We also present density functional theory calculations to characterize ideal tensile and shear strengths for these materials in order to understand how and why our developed potentials either meet or confound these expectations. 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: Improving the Computational Efficiency of Multi-Scale Modelling by Applying Model Reduction Techniques

Author(s): Malgorzata J. Zimon, *U. Strathclyde*; Prof. David R. Emerson, *STFC Daresbury Lab.*; Dr. Leopold Grinberg, *IBM T. J. Watson Rsch. Center*; Dr. Robert Prosser, *U. Manchester*; Prof. Jason M. Reese, *U. Edinburgh*.

Understanding physical phenomena across a broad range of disparate length and time scales is a very challenging task. Multi-physics simulations can provide detailed descriptions of systems driven by multi-scale events and are encountered in many scientific and engineering problems. Examples demonstrating the ubiquity of multi-scale, multi-physics applications include the dynamics of complex materials, the classical turbulence problems, meteorological predictions, chemical and biological reactions and emergent rheology. In addition, there is significant potential to apply these methods to sociological problems, such as crowd and traffic flow, and big data topics such as smart cities. Popular multi-scale modelling approaches try to couple molecular simulations to continuum dynamics. The central problem with this strategy is the accurate transfer of smooth gradients and precise particle distribution descriptions from the molecular system to continuum solver; there currently exist many sources of uncertainty and noise disturbing this intra-scale communication, with a concomitant loss of simulation fidelity. Extracting the genuine information (and hence, emergent macro-scale fields) from indirect, noisy particle measurements can be viewed as solving the statistical inverse problem, where the object of interest is not easily accessible. The presence of noise in the data can be reduced by simple averaging over a large number of samples, but the computational intensity of the model is then increased, resulting in bottlenecks in intra-scale communication. There is therefore a growing need, from both an academic and industrial perspective, for a systematic, mathematically rigorous de-noising approach in molecular-continuum simulations. In order to improve the efficiency of estimating the unknown structure from the disturbed observations, a number of model reduction techniques combined with window proper orthogonal decomposition have been applied, including singular spectrum analysis, wavelet transform, and empirical mode decomposition. The strengths and weaknesses of each procedure, and their extensions to solve statistical inverse problems for particle simulations, will be discussed. During the talk, combinations of these methods will be shown to have the capability to improve the signal-to-noise ratio and reduce the computational cost relative to standard approach.

Title: Three-Dimensional Modeling Investigation of the Parameters Controlling Re-Orientation of Hydraulic Fractures when Encountering Pre-Existing Natural Fractures

Author(s): Navid Zolfaghari Moheb, Andrew P. Bunger, *U. Pittsburgh.*

This research is conducted to study the mechanisms that determine behavior of fluid-driven fractures in interaction with pre-existing natural fractures. Specifically, we aim to consider the three-dimensional nature of these interactions, highlighting how the parameters controlling the interaction, and the various outcomes of the interaction, differ between two and three-dimensional models. We use a finite element method that centers on the implementations of zero thickness, pore pressure-cohesive zone elements to model the propagation of hydraulic fractures in naturally-fractured formations. In this modeling, the rock is assumed to be elastic and impermeable and the fluid flow is following lubrication theory. Various factors that can change the fracture propagation through the intersection were examined to predict conditions under which the hydraulic fracture will cross the natural fracture, be captured by the natural fracture, or experience a mix of the two outcomes where fluid is partitioned to both the through-going hydraulic fracture and to the natural fracture. One of the variables that can affect the capturing of the hydraulic fracture to the natural fracture is the angle of incidence, which has been explored substantially in 2D but for which much less is understood in 3D. Our model shows the interplay between the in situ stress and the 3D orientation of the natural fracture in determining how the hydraulic fracture will behavior upon intersection. Moreover, the often-ignored coupling with fluid flow, which brings in dependence of the interaction on fluid viscosity and injection rate, is shown to, in certain circumstances, have a profound impact on the hydraulic fracture behavior.

Title: Nitsche's Method for Helmholtz-Type Variational Problems with Embedded Interface

Author(s): Zilong Zou, Wilkins Aquino, *Duke U.*; Isaac Harari, *Tel Aviv U.*

In this work, we investigate the potential of Nitsche's formulation to weakly enforce the kinematic constraints at an embedded interface in Helmholtz-type problems. Such interface problems frequently arise in the analysis of steady-state dynamics of domains consisting of different materials. Allowing embedded interfaces in a FE mesh provides significant ease for discretization, especially when the material interface has a complex geometry. We provide analytical results that establish the well-posedness of the resulting Helmholtz variational problem and convergence of finite element discretizations. In particular, we derive an explicit expression of the inf-sup constant. The inf-sup constant remains positive provided that the Nitsche's stabilization parameter is judiciously chosen and that the wavenumber does not coincide with the eigenvalues of the stabilized coercive operator. We then apply our formulation to several numerical examples using simple 2D plane-wave problems that confirm our analytical findings. To this end, we demonstrate the asymptotic convergence of the proposed method and show that numerical results are in accordance with the theoretical analysis.