Abstracts for USACM Thematic Conference on Meshfree and Particle Methods: Applications and Theory Sante Fe, NM

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Contents

1 Plenary Talks

Title: The Future for Modeling Extreme Events: Exemplar Problems for Meshless Methods

Presenter: Stephen W. Attaway
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Abstract: Many challenges remain in the search for numerical models that are predictive for extreme events. This talk will provide some examples of extreme events that require a combined approach for modeling and simulation with tests and evaluation. Most structures are designed for a functional life that keeps their behavior in the linear elastic, small deformation range. When buildings are subjected to extreme loads from earthquakes, fires, or terrorist attacks, the tools used for structural designs often fail to provide a technical basis for risk. Using a combination of modeling and simulation with tests and evaluation can provide the technical basis for high-consequence decisions relative to system safety and performance margins. The emergence of exascale computers with millions of cores allows simulations of transient dynamics phenomena at unprecedented scales and fidelity. This talk will outline exemplar problems that, if solved by meshless methods, will help demonstrate the potential of these methods. The challenge problems were selected based on the availability of experiments with quality data that can be compared with simulations.

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Title: Particle Methods: A Long View

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Abstract: The history (a), unresolved problems (b), and future directions (c) for particle methods are considered. (a) The history of particle methods is already known in its essentials. Harlow's pioneering work on the particle-in-cell (PIC) method, for example, revealed the power of combined Eulerian and Lagrangian descriptions of fluid. Less well-known is that the choices Harlow made frustrated attempts to improve PIC, and that Birdsall's success in simulating plasmas kept PIC alive. Since the point in studying history is to avoid repeating it, the previously suppressed history of FLIP reminds us to remember both Harlow and Birdsall. (b) Stability and angular momentum comprise my short list of unresolved problems, but for different reasons. Harlow observed a "ringing instability" in stagnating fluid flows. Langdon analyzed a "finite grid instability" in plasma simulations. They are both caused by aliasing, and analysis shows that PIC, FLIP, and MPM are all unstable. In recent papers, Zhang describes noise caused by cell-crossing in MPM, and Teran adds dissipation to FLIP to suppress noise in modeling snow. Betti asks the inconvenient question, "How can you get useful results from a method that's always unstable?" Is there one instability or many, and is existing analysis incomplete? Particle methods conserve angular momentum. In general, finite difference methods don't, or, at least, not as well. Direct comparisons have shown this, but repetition may be necessary for acceptance. (c) Congressional redistricting and turbulence modeling are interesting problems for which particle methods have special abilities. Consider a particle calculation with fixed particles and a moving adaptive grid. Were particles to represent voters and the grid adapted to equalize the number of voters in each grid cell, how would that compare with districts presently drawn by state legislatures? Turbulence transport models are generally validated by comparison with experiments or other models. Experiments generally have more complex boundary conditions than spectral methods can accommodate, but particle methods can. Further, the Reynolds stress computed from a fine grid calculation can provide closure for a coarse grid calculation and means to determine what scales are important.

2 Mathematical Theory and Method Development

Title: Enhanced local maximum-entropy approximation for stable meshfree simulations

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Abstract: We introduce an improved meshfree approximation scheme which is based on the local maximum-entropy strategy as a compromise between shape function locality and entropy in an information-theoretical sense. The improved version is specifically designed for severe, finite deformation and offers significantly enhanced stability as opposed to the original formulation. This is achieved by - (i) formulating the quasistatic mechanical boundary value problem in a suitable updated-Lagrangian setting, (ii) introducing anisotropy in the shape function support to accommodate directional variations in nodal spacing with increasing deformation and eliminate tensile instability, (iii) spatially bounding and evolving shape function support to restrict the domain of influence and increase efficiency, (iv) truncating shape functions at interfaces in order to stably represent multi-component systems like composites or polycrystals. The new scheme is applied to benchmark problems of severe elastic deformation that demonstrate its performance both in terms of accuracy (as compared to exact solutions and, where applicable, finite element simulations) and efficiency. Importantly, the presented formulation overcomes the classical tensile instability found in most meshfree interpolation schemes, as shown for stable simulations of, e.g., the inhomogeneous extension of a hyperelastic block up to 100

Title: A machine learning enhanced data-driven simulation of solids and structures with noisy database

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Abstract: Data-driven computing in computational mechanics integrates well-established physical laws with experimental material data directly and, therefore, minimizes the necessity of phenomenological constitutive models that remain difficult in characterizing complex material behavior and calibrating model fitting coefficients. A new data-driven simulation approach based on manifold learning techniques, termed locally convex data-driven (LCDD) computing, is proposed for elastostatics problems, aiming to enhance robustness against noise and outliers in data sets and prevent unexpected suboptimal convergence. Compared with existing data-driven methods based on minimizing the distance to a single data point, LCDD seeks for optimum material solutions from a convex hull constructed locally upon the associated k-nearest neighbor (k-NN) points, which leads to less sensitivity to noisy data and ensures convergence stability. By using the penalty relaxation, the searching for optimal data is formulated as a classical minimization problem and can be solved efficiently. In addition, it is shown that LCDD performs well for high-dimensional data sets with data points that are relatively sparse. This is because the inherent manifold learning can capture the underlying structure of the material data by the reproducibility of locally linear approximation. Numerical tests in truss problems and 2D elasticity mechanics are given to validate the robustness, accuracy, and convergence properties of the proposed approach.

Title: Particle-based inelasticity vs grid-based updates in MPM

Presenter: Chad Hammerquist
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Abstract: In many MPM codes, the stress and strain tensors are calculated incrementally on the particles. Since the stress and strain fields on the particle basis are never synced with the grid, these fields can develop high frequency spatial oscillations that are not seen by the grid basis. Because these modes of oscillations are not seen by the grid, they don't generally have a significant effect on the grid solution. However, in analyses using inelastic constitutive laws, such as with plasticity or damage, the particle stresses could be needed to calculate the onset of inelasticity and evolution of damage or plastic strains. These constitutive law calculations are done on the particle using the particle stresses. Subsequently, any unphysical high stress on a single particle from oscillations could cause that particle to behave (yield, damage, or fail prematurely) unphysically, eventually degrading the accuracy of the overall analysis. Effects and causes of these stress oscillations, along with exacerbating conditions are investigated. Several methods to mitigate this problem are presented. Results are demonstrated with simulations involving damage mechanics.

Title: A stable SPH discretization of the elliptic operator with heterogeneous coefficients

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Abstract: Smoothed particle hydrodynamics (SPH) has been extensively used to model high and low Reynolds number flows, free surface flows and collapse of dams, study pore-scale flow and dispersion, elasticity, and thermal problems. In different applications, it is required to have a stable and accurate discretization of the elliptic operator with homogeneous and heterogeneous coefficients. In this paper, the stability and approximation analysis of different SPH discretization schemes (traditional and new) of the diagonal elliptic operator for homogeneous and heterogeneous media are presented. The optimum and new discretization scheme is also proposed. The new scheme enhances the Laplace approximation (Brookshaw's scheme (1985) and Schwaiger's scheme (2008)) used in the SPH community for thermal, viscous, and pressure projection problems with an isotropic elliptic operator. The sufficient monotonicity condition is also formulated leading to the constraint on the kernel shape and particles distribution. The numerical results are illustrated by numerical examples, where the comparison between different versions of the meshless discretization methods are presented.

Title: Local Lagrange Functions and the BBO paradigm

Presenter: Joe Ward
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Co-Author 1: Francis Narcowich; Texas A&M University

Abstract: Local Lagrange Functions and the BBO Paradigm J. D. Ward In their 2003 paper "Survey of Meshless and Generalized Finite Element Methods: A Unified Approach", Babuska, Banerjee and Osborne outlined a general program and basic properties that any good meshless or GFEM method should possess. In this talk, we will focus on trial (approximation) spaces whose bases consist of local Lagrange functions constructed using polyharmonic or Matern kernels. While not compactly supported, such functions are known to be extremely well localized and scale with the point spreads. An easy to construct quasi-interpolation operator implements the approximant associated with the trial spaces. The underlying compact domain can either be with or without boundary. We will discuss the various approximation properties that these spaces are known to possess in terms of the BBO paradigm. The talk is based on a number of papers with various authors including E. Fuselier, T. Hangelbroek, F. J. Narcowich, C. Rieger, X. Sun and G. Wright.

Title: A Stable Generalized/eXtended FEM with Discontinuous Interpolant for Fracture Mechanics

Presenter: Alfredo Sanchez-Rivadeneira
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Abstract: The successful development of a optimally convergent Generalized FEM (GFEM) with conditioning not worse than FEM for fracture mechanics problems has been mostly limited to first-order accurate approximations. Numerical studies with three classes of quadratic GFEM approximations are presented, showing errors that are orders of magnitude smaller than the FEM with quarter-point elements, which in general is not the case for first order GFEM approximations. However, all of them lead to severely ill-conditioned system of equations. Enrichment modifications able to address the ill-conditioning of quadratic GFEM approximations while preserving their optimal convergence are proposed. A robust enrichment modification strategy based on a discontinuous finite element interpolant is proposed to control the conditioning of branch function enrichments, while a combination of enrichment shifting by its nodal value and a local finite element mesh modification in the neighborhood of the crack surface is used to address the lack of robustness of Heaviside enrichments. The discontinuous FE interpolant is a generalization of the continuous one used with the Stable GFEM (SGFEM). It is shown that SGFEM spaces based on p-hierarchical FEM enrichments are the same as their GFEM counterparts. This guarantees that both GFEM and SGFEM spaces will lead to the same solution, which is not the case for the other classes of second-order spaces. The robustness of the proposed approximation spaces with respect to the position of the mesh relative to the crack is also demonstrated numerically.

Title: Localized high-order meshfree methods for semi-Lagrangian advection on surfaces

Presenter: Grady Wright
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Abstract: We present a new meshfree semi-Lagrangian method for simulating advection on two-dimensional surfaces embedded in three-dimensional space. The method is based on localized radial basis function (RBF) interpolation using polyharmonic splines with polynomials, formulated in the tangent space of the surface. The semi-Lagrangian framework allows the method to avoid the use of any stabilization terms (such as hyperviscosity) during time-integration, thus reducing the number of parameters that have to be tuned. Additionally, time-steps that exceed CFL condition can be used without suffering from temporal instabilities. Finally, the method is formulated in Cartesian coordinates, avoiding any artificial singularities that arise from surface-based coordinates. We illustrate the accuracy and stability of the method by solving several example problems on various surfaces. We also discuss the extension of these methods to more general advection-reaction-diffusion equations.

Title: An asymptotically compatible meshfree quadrature rule for nonlocal problems with applications to peridynamics

Presenter: Huaiqian You
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Abstract: We present a meshfree quadrature rule for compactly supported nonlocal integro-differential equations (IDEs) with radial kernels. We apply this rule to develop a meshfree discretization of a peridynamic solid mechanics model that requires no background mesh. Existing discretizations of peridynamic models have been shown to exhibit a lack of asymptotic compatibility to the corresponding linearly elastic local solution. By posing the quadrature rule as an equality constrained least squares problem, we obtain asymptotically compatible convergence by introducing polynomial reproduction constraints. Our approach naturally handles traction-free conditions, surface effects, and damage modeling for both static and dynamic problems. We demonstrate high-order convergence to the local theory by comparing to manufactured solutions and to cases with crack singularities for which an analytic solution is available. Finally, we verify the applicability of the approach to realistic problems by reproducing high-velocity impact results from the Kalthoff-Winkler experiments.

Title: Conservative Meshfree Discretization

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Abstract: Discrete conservation principles have proven elusive to particle discretizations without the aid of a background mesh. This may be understood in the context of the generalized Stokes theorem; momentum conservation follows from a relationship between cell integrals and face fluxes, while particle methods traditionally are defined purely in terms of point evaluation functionals. We illustrate how generalized moving least squares may be used to generate classical quadrature schemes on a mesh, and then present a new meshfree virtual divergence theorem. We present several schemes for a variety of applications where these conservation principles provide favorable properties in both an Eulerian and Lagrangian setting.

Title: Kernel-based reconstruction methods for uncertainty quantification

Presenter: Christian Rieger
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Abstract: The field of uncertainty quantification (often in connection with parametric operator equations) has gained an increasing attention over the last years.

For a parametric operator equation and a related quantity of interest (QoI), one is often interested in evaluating the QoI at a parameter value from known values of the QoI at some other parameter values. In practice such an approach is motivated by the usually high cost to predict the QoI directly by solving the operator equation. Moreover, one is often interested in "good" parameter values where the direct computation will lead to the biggest knowledge gain. Both questions can be formalized mathematically as usually high dimensional reconstruction problems.

In this talk we will present kernel based methods for such reconstruction problems. We will discuss also their relation to Gaussian process regression which will be especially useful for the second question about the best possible design of evaluation parameters.

We will discuss recent progress on localized bases to decrease the computational complexity of kernel based methods.

Title: Moving-least-squares based extrapolation and local Lagrange approximation

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Abstract: En this talk we will discuss the following extrapolation problem. Suppose only that we only know the values of a C^{M+1} function $f : \Omega \to \mathbb{R}$ on a finite, quasi-uniform set X of centers in a bounded domain $\Omega \subset \mathbb{R}^d$. Using various approximations methods, rates of approximation for f in the interior of Ω – i.e., points $x \in \Omega$ such that $dist(x, \partial\Omega) \geq \varrho \geq 0$ – are known to be optimal. Why? Values of f at an interior point x are "pinned down" by centers that are quasi-uniform in a ball centered at x. However, for x near $\partial\Omega$, the centers are *not* quasi-uniform in a ball about x, just in the half neighborhood of x that is farthest from Ω, with only a few points coming from the half closest the boundary. This causes the approximation to degrade near $\partial\Omega$. One way of ameliorating this problem is to turn Ω into the interior of a larger domain $\widetilde{\Omega}$, and extrapolate f, or rather the values of f, to a finite, quasi-uniform set of points $Y \in \widetilde{\Omega} \setminus \Omega$, in such a way that an approximation corresponding to centers in $X \cup Y$, when restricted to Ω, retains the same rates near the boundary as in the interior. Here, we present a moving-least-squares method for extrapolation and approximation method base on thin-plate spline Local Lagrange functions.

Title: Implicit Gradient for Numerical Solution of PDEs

Presenter: J.S. Chen
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Abstract: Implicit gradient (IG) is expressed in an integral equation with embedded gradient consistency without explicit derivatives. It offers a paradigm for constructing approximations of function derivatives for the numerical solution of PDEs, either by using strong forms or weak forms. A straightforward application of IG is for the gradient-type regularization of ill-posed problems, such as strain localization problems. IG can also be used to construct stabilization of convection dominated problems and as the stabilization of nodally integrated Galerkin equations. Without the need of taking directives of approximation functions, IG also offers computational efficiency for Meshfree-based numerical solutions of PDEs. This talk will introduce continuous and discrete IG for approximation of derivatives, discuss the gradient consistency of IG and its convergence properties in solving PDEs, and demonstrate its applications to strain localization, convection dominated problems, and modeling of damage and fracture processes in solids subjected to extreme loadings.

Title: A finite volume reproducing kernel particle method

Presenter: Saili Yang
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Abstract: A significant amount of progress has been made in developing Meshfree method during the past 20 years in solving PDEs. Meshfree methods can be generally categorized into two branches: the Galerkin meshfree methods based on the weak form and the collocation meshfree methods based on the strong form [1]. However, due to numerical integration of the weak form, instability and loss of convergence are two key issues which require special treatments [2]. The essential boundary conditions cannot be imposed directly as well and also require special techniques. Strong form based meshfree methods do not have these issues, but they do require the use of expensive higher order derivatives [3]. A finite volume method based on the reproducing kernel approximation is introduced in the current work, as an alternative to current meshfree implementations. Starting from the global Petrov-Galerkin method, a conforming Heavyside function is chosen as the test function. The divergence theorem is used to simplify the implementation, which avoids higher order derivatives. Due to this process, the variational consistency conditions are also inherently satisfied, and the method can attain optimal convergence rates. Furthermore, the essential boundary conditions can be directly imposed, and no instability is observed. Several benchmark examples are presented to show the accuracy, convergence, and stability of the method, and overall effectiveness versus current weak- and strong-form based meshfree methods is assessed. Keywords: Reproducing kernel approximation; Finite volume method; Variational consistency conditions; Meshfree methods; References: 1. Chen J.S., Hillman M, Chi S-W. Meshfree Methods: Progress Made after 20 Years. J Eng Mech. 2017;143(4):04017001. doi:10.1061/(ASCE)EM.1943-7889.0001176. 2. Chen J.S., Wu C, Yoon S. A stabilized conforming nodal integration for Galerkin mesh-free methods. Int J Numer Meth Eng. 2001;0207(February 2000):435-466. doi:10.1002/1097-0207(20010120)50. 3. Hu H-Y, Lai C-K, Chen J.S. A study on convergence and complexity of reproducing kernel collocation method. Interact multiscale Mech. 2009;2(3):295-319. doi:10.12989/imm.2009.2.3.295.

Title: Consistent Strong Enforcement of Essential Boundary Conditions in Meshfree Methods

Presenter: Kuan-Chung Lin
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Abstract: Essential boundary conditions are non-trivial to be enforced in most Galerkin meshfree methods due to the lack of the Kronecker delta property in the approximation. Commonly used approaches to strongly enforce the boundary conditions include the so-called transformation method [1], boundary singular kernel method [2], and reproducing kernel approximation with interpolation property [3]. However, with these methods, the approximation spaces in the general case are not strictly kinematically admissible, as the enforce boundary values can actually deviate between nodes. In this work, it is shown that for meshfree approximations with completeness higher than linear, the associated optimal convergence rates are not obtained with the strong enforcement of boundary conditions at nodes. Two new weak forms are introduced to remedy this difficulty, which allow for the inadmissibility of the test function, or both the test and trial function. Several benchmark problems are solved to demonstrate that optimal convergence rates can be restored using the proposed method. In addition, it is shown that the formulation allows improved accuracy using both traditional and non-traditional techniques: increasing bases order (p-refinement), decreasing nodal spacing (h-refinement), and by increasing dilation (a-refinement).

References: [1] Chen, J.S., Pan, C., Wu, C.T., Liu, W.K., 1996. Reproducing kernel particle methods for large deformation analysis of non-linear structures. Computer Methods in Applied Mechanics and Engineering, Vol. 139(1-4), pp.195–227. [2] Chen, J.S., Wang, H.P., 2000. New boundary condition treatments in meshfree computation of contact problems. Computer Methods in Applied Mechanics and Engineering, Vol. 187(3-4), pp. 441–468. [3] Chen, J.S., Han, W., You, Y., Meng, X., 2003. A reproducing kernel method with nodal interpolation property. International Journal for Numerical Methods in Engineering, Vol. 56(7), pp. 935–960.

Title: Generalized Reproducing Kernel Peridynamics

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Abstract: Recently, a connection has been established between state-based peridynamics [1] and the reproducing kernel particle method [1] with implicit gradients, based on an analysis of the two methods in a uniform discretization, away from the influence of the boundary [3]. In this work, the relationship is established in a general, non-uniform setting, fully illuminating the commonality and differences between the two methods. It is then shown that the similarities enable the approximation of gradients to be generalized under a framework which encompasses both methodologies. Leveraging the newly-discovered connections, a new method called Generalized Reproducing Kernel Peridynamics is proposed where arbitrary-order accuracy and associated optimal convergence rates can be obtained. It is shown that these properties can be achieved using only nodal integration as well. Several benchmark problems are solved to verify the arbitrary high-order accuracy and demonstrate optimal convergence of the proposed method.

Title: Generalized Moving Least Squares: Approximation theory and applications

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Abstract: In this talk we present existence and approximation results for the reconstruction of a few classes of linear functionals, including differential and integral functionals, using the Generalized Moving Least Square (GMLS) method. These results extend or specialize classical MLS theoretical results, and they rely both on the classic approximation theory for finite elements and on existence/approximation results for scattered data. In particular, we will consider the reconstruction of vector fields in Sobolev spaces and the reconstruction of differential k-forms. We show how these results can be applied to a variety of meshless schemes such as staggered stable discretizations for diffusion and elasticity problems.

3 Multi-Scale

Title: Multicomponent Molecular-Continuum Simulations Using Smoothed Dissipative Particle Dynamics

Presenter: Nikolai D. Petsev
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Abstract: Understanding a broad spectrum of multiscale problems in molecular and interfacial physics requires simulations able to span molecular to mesoscopic scales. Due to this challenge, we have developed a multiscale simulation framework that couples mesoscale hydrodynamic models using a stochastic particle-based technique called "smoothed dissipative particle dynamics" (SDPD) to molecular domains using conventional molecular dynamics (MD) simulations. Using this multiscale strategy, it is possible to embed a MD region within a hierarchy of SDPD continuum domains, incrementally characterized by larger and larger length scales that allow simulations spanning the atomistic to the non-fluctuating hydrodynamic limit. In addition, we describe a novel generalization of these approaches to multicomponent systems and hence provide a major step towards modeling multiscale phenomena involving one or more dissolved species. Finally, we outline some future directions, including systems featuring chemical reactions.

Title: A Scale-Bridging Generalized Finite Element Method for Parallel Simulations of Spot Welds in Large Structures

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Abstract: Spot welds are commonly used to join thin gauge metallic structural components of automotive and aerospace vehicles. The stiffness of these components is strongly dependent on the design of their sub-component connections. Multi-point constraints are commonly used to represent spot welds in finite element models. However, they lead to mesh-dependent solutions and provide no useful information about the stresses around the spot weld, which are needed for life prediction of the connection.

In this talk, we present a Generalized Finite Element Method (GFEM) based on the solution of interdependent macro/global and fine/local scale problems. The local problems focus on the resolution of fine-scale features of the solution near regions with singularities or localized nonlinearities, while the global problem addresses the macro-scale behaviour of the structure. Fine-scale solutions are accurately computed in parallel using the h-version of the GFEM and embedded into the global solution space using the partition of unity method. Thus, the proposed method does not rely on a-priori knowledge about the solution of the problem. Other numerical methods such as the Isogeometric Analysis, Peridynamics, etc., can also be used to solve the local problems. This GFEM enables accurate modeling of problems involving nonlinear, multi-scale phenomena on macro-scale meshes that are orders of magnitude coarser than those required by the FEM. Numerical examples show the scalability of the method on shared memory computers and a comparison in terms of computational performance and accuracy, with a direct finite element solver. Application of the method to the simulation of a representative hypersonic aircraft panel with a large number of spot welds is presented.

Title: An Immersed Reproducing Kernel Particle Method For Modeling Inhomogeneous Media

Presenter: Frank Beckwith
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Abstract: The simulation of problems involving inhomogeneous media or material interfaces often involve complex geometries. For body-fitted methods such as the finite element method (FEM) these problems are tedious to discretize due to the conforming requirements at the material interface, leading to poor quality elements and meshes. The Reproducing Kernel Particle Method (RKPM) does not suffer from such discretization constraints, but fails to capture weak discontinuities at material interfaces without explicit enrichment. An immersed Reproducing Kernel Particle Method is proposed to model the complex reinforcement geometry using an immersed domain approach. The compatibility conditions on the material interfaces are enforced via Nitsche's method with embedded equilibrium. This approach allows independent approximations and discretizations for the background matrix and the foreground inclusion, and naturally yields strain jumps across the material interfaces. The reproducing kernel (RK) approximations and discretizations of both foreground and background domains are considered in this work due to their adjustable regularity [1], but other approximations such as the finite element method can also be employed under this framework. Several numerical examples are presented to examine the effectiveness of the proposed method.

References:

[1] J.S. Chen, M. Hillman, and S.-W. Chi. Meshfree methods: Progress made after 20 years. Journal of Engineering Mechanics, 143(4):04017001, 2017.

Title: Multi-scale modelling of granular pile collapse by using material point method and discrete element method

Presenter: Chuanqi Liu
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Abstract: Granular debris flows are often observed in mountainous areas in Southwestern China. The process is accompanied with large deformation and the evident transitions between solid- and fluid-like states bring difficulties in proposing a unified phenomenological constitutive model. In this study, a hierarchical multi-scale modelling scheme is developed to simulate a granular pile collapse. The macroscopic behaviour is modelled by using material point method (MPM), which is suitable for large deformation, while the constitution relation at each material point is extracted from discrete element method (DEM) modelling. This MPM/DEM multi-scale modelling strategy abandons constitutive models as required in MPM, and facilitates effective cross-scale interpretation and understanding of granular flow behaviour. It helps to simulate the large deformation of granular materials when their constitute relations are hard to be derived explicitly.

Title: Non-Isothermal Smoothed Dissipative Particle Dynamics

Presenter: Nikos Gatsonis
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Abstract: An overview is presented of a non-isothermal Smoothed Dissipative Particle Dynamics model and its implementation with dynamic virtual particle allocation (SDPD-DV) for liquids and gases in arbitrary wall-bounded domains. The particle entropy for monatomic and diatomic gases, is evaluated through a Sackur-Tetrode type of equation, which in turn provides the internal energy. For liquids, the entropy and the internal energy are given as a second-order expansion using the coefficient of volumetric thermal expansion and of adiabatic compressibility. The fluid particle pressure and temperature are calculated by thermodynamic relations. The integration of position-momentum SDPD-DV equations was accomplished with a velocity-Verlet (VV) algorithm. Bounce-forward is added to the velocity-Verlet integrator when needed to fully prevent particle penetration. The integration of the entropy SDPD-DV equation is accomplished with an implementation of the Runge-Kutta algortihm. The dynamic virtual particles allow the implementation of Dirichlet and Neumann thermal boundary conditions. The sampling methods used in SDPD-DV for particle, fluid (macroscopic) properties, hydrodynamic fluctuations, the self-diffusion and viscosity coefficients are presented. The theoretical hydrodynamic fluctuations are summarized. A series of SDPD simulations of gaseous nitrogen and liquid water flows in planar minichannels with heat conduction are presented and the results are compared with analytical and numerical solutions. An extensive set of SDPD-DV simulations of liquid water, argon gas and diatomic nitrogen gas is presented and the SDPD-DV derived density, temperature, pressure, self-diffusion coefficient, shear viscosity, and hydrodynamic fluctuations are compared with analytical and experimental values.

Title: Applications of Discrete Element Method (DEM) in Micromechanical modeling of Materials

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Abstract: Modeling and simulation across multiple length scales of materials is important in predicting material performances in service loading, and in designing materials for specific applications. Micromechanical modeling has been performed to gain understanding on the structure-property relationship of materials at microstructural level. Different materials have different microstructures, and different methods are chosen to best capture the fundamental physics of the material at this scale. Some biological materials and cementitious materials have microstructures which are intrinsically discrete in nature. DEM method can be applied to model these materials at the microscale. Here we present two examples of such applications. The microstructure of nacre of abalone shells were modeled with DEM method. The aragonite mineral tablets were modeled with different shapes of three dimensional polygon particles to represent the Voronoi like patterns of mineral tablets assembly observed in experiments. The organic matrix was modeled with a group of spring elements and mineral bridges modeled with elastic bonds. The models investigate the effects of mineral bridges, organic matrix and three dimensional microstructure architecture on the damage and crack propagation mechanisms of nacre, providing insight into the design of nacre-inspired materials. Calcium-Silicate-Hydrate (C-S-H), the most important hydrate phase in cementitious materials, was modeled with discrete element method (DEM). The inter-particle forces consisted of traditional friction and contact forces with the addition of nanometer scale forces such as van der Waals and ionic correlation forces. Monte Carlo (MC) simulations were performed to estimate the ionic correlation forces between C-S-H nanoparticles. The models simulated the nanoindentation experiments of C-S-H to investigate the effects of nanoparticle packing, nanoparticle morphology, interparticle forces and nanoparticle properties on the deformation mechanisms and mechanical properties of C-S-H matrix. Permission to publish was granted by the Director, ERDC Geotechnical and Structures Laboratory.

Title: A Partition Of Unity Method using fine-scale enrichments

Presenter: Denis Dusseldorf
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Abstract: The simulation of the responses of multimaterials in the context of classical Finite Element Analysis poses severe problems. Since the properties of the employed materials can vary strongly, the gradients of the solution feature substantial discontinuities at inclusion interfaces. In the presence of fine scale features (such as fibers), the underlying mesh needs to be highly refined in order to obtain accurate approximations. To avoid very large numbers of degrees of freedom, either the discontinuous material coefficients are replaced by homogenized smooth coefficients, or the shape functions are replaced by numerically computed functions that already show the desired behaviour on the fine scale. We present a Partition of Unity Method that makes use of a class of well-suited enrichments that drastically improve the performance of the method. The problem of two dimensional linear elasticity is discussed and numerical results are presented. An extension to three dimensional laminates is given.

Title: A Concurrent Multiscale Approach tto Coupled Peridynamic/FEM Simulation

Presenter: Dong Qian
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Abstract: A concurrent multiscale computational approach that integrates the space-time finite element method and peridynamics is presented. First, a space-time enrichment method [1] is established based on the time discontinuous Galerkin framework. Specifically, the enriched approximation is constructed by augmenting the regular space-time FEM shape functions with enrichment that represents the final scale physics. We then introduce the peridynamics (PD) framework to capture the fine scale phenomenon such as crack initiation and propagation. The space-time FEM and PD simulations are performed concurrently and integrated through the bridging scale concept. The second aspect of the implementation involve the treatment of the interface boundary between space-time FEM and PD that is based on a nonlocal version of the Matching Boundary Condition (MBC) [2]. The MBC is cast in the form of parameterized expressions involving displacements and their higher-order time derivatives of the peridynamic (PD) nodes at the numerical interface. The corresponding parameters are solved by zeroing the associated residual and its higher order derivatives that are functions of the dispersion relation at the particular wave length of interest. The goal is to eliminate any artificial wave reflection at such a numerical interface and realize a matching of the dispersive properties. Implementation of MBC in both simple 1D and higher dimensional cases will be discussed with extensive validation. Finally, we illustrate the robustness of the approach by comparison with direct numerical simulation. Example problems that involve brittle fracture propagation will be presented.

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Title: Deep-reinforcement-learning-enhanced computational failure mechanics across multiple scales

Presenter: WaiChing Sun
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Abstract: This paper presents a new conceptual framework to employ refinement Q-learning technique to generate constitutive responses for interfaces. We simplify the process of writing constitutive laws as a sequence of actions made with the goal of maximizing the reward, a function of accuracy, robustness and forward prediction quality. With the well defined objective, state, action, rule and reward, we then introduce a deep reinforcement Q-learning process to automate the modeling writing process. By formulating the reinforcement learning as a Markov decision process and using neural network to estimate the Q function, the computer agent is able to self-improve the constitutive model it generated through self-playing, in the same way AlphaGo (the algorithm that outplayed the world champion in the game of Go)improves the action through self-playing. Our numerical examples show that the resultant model is not only outperform the benchmark traction-separation laws, but is also capable of detecting hidden mechanisms that are difficult to incorporate manually and find ways to incorporate them to improve the accuracy of the forward predictions.

Title: SPH Model for Nanoscale Multiphase Flows

Presenter: Alexandre Tartakovsky
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Abstract: We propose a nonlocal model for surface tension. This model, in combination with the Landau-Lifshitz-Navier-Stokes equations, describes mesoscale features of the multiphase flow, including the static (pressure) tensor and curvature dependence of surface tension. The nonlocal model is obtained in the form of an integral of a molecular-force-like function added into the momentum conservation equation. We present an analytical steady-state solution for fluid pressure at the fluid-fluid interface and numerical Smoothed Particle Hydrodynamics solutions that reveal the mesoscopic features of the proposed model.

Title: Coupling Methods in Peridynamics for Effective Failure and Damage Simulation

Presenter: Pablo Seleson
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Abstract: Predictive failure and damage simulation has been a topic a fundamental interest in materials science and engineering. A recently developed nonlocal theory called peridynamics has been a subject of increased interest in the computational mechanics community, due to its ability to naturally represent material discontinuities and handle complex dynamically evolving cracks. However, peridynamic simulations are significantly computationally more expensive than their classical (local) continuum mechanics analogues. Consequently, it is of interest to develop effective coupling methods with the capability to seamlessly combine nonlocal and local models. In this presentation, we will discuss methods to couple peridynamics and classical elasticity, and we will demonstrate the effectiveness of those methods through numerical simulations.

Title: Advances in a multiscale generalized FEM for large-scale simulations

Presenter: Julia Plews
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Abstract: This presentation will explore advances in data- and task-parallel aspects of the generalized finite element method with global–local enrichment functions (GFEMgl) for large-scale, multiscale computational mechanics simulations. The GFEMgl simultaneously resolves fine-scale (e.g., crack- or material-scale) and coarse-scale (e.g., component- or structural-scale) physics in interdependent local and global boundary value problems. Local numerical solutions arising from a discretization approach of the user's choosing are inserted into the global basis as enrichment functions to achieve strong coupling of fine- and coarse-scale response without sacrificing fine-scale fidelity. Local problems in the GFEMgl allow the global model to maintain a similar accuracy level to direct simulations and, moreover, are embarrassingly task-parallel, yielding good scalability on shared memory computers [1,3]. However, scalable algorithms for real simulations on the next generation of manycore high-performance computing platforms must exploit a combination of data- and on-node thread-, or MPI+X, parallelism. This talk will focus on (i) a new data-parallel strategy for the GFEMgl along the lines of [2], and (ii) a hierarchical version of the GFEMgl for task-parallel resolution of multiple spatial scales. References [1] D.-J. Kim, C. Duarte, and N. Sobh. Parallel simulations of three-dimensional cracks using the generalized finite element method. Computational Mechanics, 47(3):265–282, 2011. [2] M. Mosby and K. Matouš. Computational homogenization at extreme scales. Extreme Mechanics Letters, 6:68–74, 2016. [3] J. Plews and C. Duarte. Bridging multiple structural scales with a generalized finite element method. International Journal for Numerical Methods in Engineering, 102(3–4):180–201, 2015.

4 Comparison of Related Methods

Title: Improving the integration accuracy of the material point method

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Abstract: The material point method (MPM) has been applied in the simulation of a wide variety of problems involving large material deformations, such as the modeling of granular flows [1], void growth and material failure [2], and impact [3]. The MPM employs both Lagrangian material points and a background Eulerian mesh to seek a weak solution of the partial differential equations. Unlike the finite element method (FEM), a material point is not fixed to any one element, but is free to move throughout the mesh, carrying all state information including the deformation history. During each time step, information is mapped between the material points and the mesh nodes. Since the background computational mesh is fixed, the MPM avoids both the issues of mesh entanglement in pure Lagrangian methods in cases of large deformation and numerical diffusion of history-dependent information in Eulerian methods.

The original MPM uses the material points as the integration points to perform a low-accuracy Riemann sum as the integration for the nodal force, instead of using the Gauss points as in a traditional FEM. This integration method causes the reduced accuracy and particle cell-crossing noise. The methods of reducing the cell-crossing noise have been studied extensively. In the present work we focus on improving the integration accuracy. The method developed here is independent of, although is easily combined with, the dual domain material point method to treat the cell-crossing noise; therefore, we only consider the improved integration scheme in examples of small deformation.

We first investigate the properties of accuracy and convergence of the numerical solution using either a MPM or FEM formulation for two different simple quasi-static problems: a two-dimensional (2D) linear elastic split cylinder (Brazilian disk), and a 2D elastic cantilever beam. For both formulations we use an explicit in time integration scheme with dynamic relaxation to calculate the equilibrium configurations and compare our results with an implicit algorithm. We then use the sub-point method to separate the integration points and the material points. In the sub-point method, the number of integration points is increased, while the number of material points, at which the stress is evaluated, is kept constant to avoid an increase in computational cost related to the calls to the constitutive relations [4]. We show that the sub-point method improves the numerical integration

accuracy.

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Title: A reproducing kernel enhanced approach for peridynamic solutions

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Abstract: Peridynamics is a nonlocal reformulation of continuum mechanics in which balance laws are computed through integration rather than differentiation [1]. For this reason, the peridynamic theory does not require any assumptions on the spatial differentiability of the displacement fields and remains valid in the presence of displacement discontinuities. Peridynamics is thus directly applicable to problems involving material failure and damage. The two most common discretization methods for peridynamic models used in engineering problems are the Finite Element method, based on a weak formulation and a meshfree method, based on nodal integration of the strong form. The former is computationally expensive and limited by the need of adapting the mesh to track evolving cracks. The latter approach discretizes peridynamic domains by a set of nodes, each associated with a nodal cell with a characteristic volume, leading to a particle based description of continuum systems. The behavior of each particle is then considered representative of its cell, limiting the convergence rate to first-order [2]. This work proposes the use of a meshfree Reproducing Kernel (RK) approximation [3] to the field variables in the peridynamic equations in order to increase the order of convergence of peridynamic numerical solutions. In this work, the peridynamic framework and the RK approximations are reviewed, the proposed approach is presented and the improved convergence rates in static peridynamic problems obtained using the proposed method is shown through numerical examples.

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Title: Comparison of Molecular Dynamics (MD) with Multiscale Crystal Defect Dynamics (MCDD) for Crystal Plasticity Modelling

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Co-Author 2: Bo Ren; University of California, Berkeley

Additional Co-Author(s): Wu, C.T.; Livermore Software Technology Corporation

Abstract: Understanding the mechanism of plasticity has been a critical issue in material design, manufacturing process and other engineering applications. Accordingly, crystal plasticity plays an important role in determining material properties at macroscale and it is governed by the collective behavior of large ensembles of defects such as dislocations and vacancies in crystalline materials. Molecular dynamics (MD) has been extensively used to study the isolated interaction mechanisms, but its applications are limited by the spatial and temporal resolution. In this talk, a multiscale crystal defect dynamics (MCDD) model is developed to establish a molecular-based multiscale method to achieve desired accuracy as well as affordable computational costs in crystal plasticity modelling. Specifically, a scalable multiscale defect mechanics model is constructed systematically and rigorously based on the microstructure of the original perfect crystal lattice, which bridges the scale gap between molecular dynamics and continuum modelling. MCDD model is validated by comparisons with numerical results of MD. The efficiency of MCDD method allows us to simulate dynamic evolution of defects at large scale while taking into account atomistic information. Numerical simulations show that MCDD model can simulate inelastic deformation, anisotropic plasticity and the formation of shear band, which may establish a computational statistical mechanics-based crystal plasticity paradigm and have broader impacts on understanding inelastic constitutive relations of materials in applications of high strength and high-performance structures under extreme loading conditions.

Title: A comparison of mesh-free and mesh-based Lagrangian approximations of a manufactured shear-dominated deformation field

Presenter: Joseph Bishop
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Abstract: Meshfree methods for solid mechanics have been in development for over 25 years. Initial motivations included alleviation of the burden of mesh creation and the desire to overcome the limitations of traditional mesh-based discretizations in extreme-deformation applications. Here, the approximation accuracy and robustness of both mesh-free and mesh-based Lagrangian approximations are compared using a manufactured shear-dominated deformation field. Quantitative error assessments are presented in both the L2 and H1 norms. Concepts for enabling mesh-free adaptivity are also presented.

Title: Computational modeling of joint failure using finite element and meshfree methods

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Co-Author 1: Wei Hu; LSTC

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Additional Co-Author(s): Huang Li, Ford Motor Company, China

Abstract: A car structure generally consists of hundreds of fabricated sheet metal panels and frames joined together, using a combination of different jointing techniques such as spot welding, riveting, clinching, hinging, screwing, etc. Those joints are often considered the weakest points as regards to structural strength. Therefore it is very important to understand the mechanical behavior of joints and their failure characteristics in a car design phase.

Several computational challenges are involved in modeling joint failures. First, the typical tied-contact approach would have a strong restriction to provide an accurate geometrical description of the joint model. Therefor, a sufficient meso-scale model characterizing the baseline of a joint structure is eventually needed. This leads to the second computational challenge to be resolved in the inconsistent topological coupling between solid and shell elements. Apparently, it will be computationally prohibitive to replace shell elements in the whole car body by solid elements using matching (conforming) meshes. The sub-modeling technique which commonly used in small deformation analysis is obviously not an option for the joint failure analysis. Other coupling approaches based on the non-intrusive method requires an iterative process between meso and macro computations, thus not suitable for explicit dynamics analysis in crashworthiness. Compared to previous challenges, the non-convergent material failure results of finite element methods also pose other significant problems. Specifically, the C1-continuity assumption in most finite element methods is unable to describe the kinematic discontinuity of displacement fields for material separation. Although the element deletion technique can be employed to reduce excessive straining and mesh tangling problems caused by the C1-continuity assumption, it gives another instance of numerical instability associated with the loss of conversion properties in mass and linear momentum. As a consequence, the numerical result could become very problematic and parameter sensitive. To circumvent this problem, a stable and convergent numerical method for large deformation and material failure analysis of joint models will be acquired.

In this presentation, we first provide an overview of current industrial approaches in joint failure analyses. We then present a two-scale computational technique based on

the meshfree method that overcomes those computational challenges in current industrial approaches. Finally several joint failure analyses are studied to verify the effectiveness of the proposed method. Their applications to the full car crashworthiness will also be discussed.

Title: A Comparison Study on Peridynamic Models Using Irregular Non-uniform Spatial Discretization

Presenter: Hailong Chen
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Abstract: The applicability of peridynamic models to problems with irregular non-uniformly discretized solution domain is critical. With a few exceptions, most previous peridynamic applications employ regular uniform discretization of the solution domain. Although regular uniform discretization is easy to generate, it can result in excessive computational expense because the refinement level is driven by the maximum refinement needed anywhere in the solution domain. On one hand, Local refinement is an obvious solution to this issue – concentrating material points at the locations where they are most needed for solution accuracy. On the other hand, local refinement may bring in the issue of unbalanced interaction, i.e., ghost force effect. Computational cost is not the only drawback to regular discretization, however, as they may influence crack paths due to dependencies on the orientation of the grid. Moreover, regular discretization may influence damage initiation sites because of grid symmetry and inaccurate geometry representation in the computational model. These phenomena are particularly evident when considering domains with complex or curved geometries. To overcome these aforementioned shortcomings, capability of applying peridynamic models to irregular and non-uniform spatial discretization with varying horizon size becomes critical. In this presentation, a systematic comparison on results predicted by different bond-based and state-based peridynamic models for irregular non-uniform spatial discretization will be performed. Modeling fracture of solids is out of the scope of current study, since valid peridynamic failure criterion for irregular spatial discretization is still under development and application of regular uniform grid based critical bond stretch criterion for irregular non-uniform discretization is arguable. This presentation will be organized as follows: firstly, different peridynamic models that is used in this study will be reviewed. These models includes bond-based models using conventional constant parameters and variable parameters, ordinary state-based models using conventional constant parameters and variable parameters, conventional correspondence model stabilized with spring-like force, and self-stabilized bond-associated correspondence model. Following this, the prediction and comparison among these models using three different types of problems will be presented. Discussion and conclusion are drawn based on the current study.

Title: Meshfree cohesive phase-field peridynamics

Presenter: Michael Tupek
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Abstract: A novel approach for modeling material failure, fracture, and separation is presented. After identifying the relation between cohesive, phase-field and peridynamic representations of fracture, we leverage and combine the best ideas from these fields to formulate a novel meshfree fracture approach. Features of the proposed approach include: true material separation, no mass loss, energy dissipation proportional to crack surface area, minimal computational geometry, mesh convergence, parallel scalability, and a regularization length scale which is independent of the fracture length scale.

5 Rapid Design-to-Analysis

Title: Application of the Conformal Decomposition Finite Element Method for Rapid Turnaround Analysis of Tomographic Imaging and Particle Simulation Based Mesostructures

Presenter: Scott Roberts
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Abstract: Composite materials are often comprised at the mesoscale of particles, fibers, or other structures embedded within a matrix material. A prime example of this is in lithium-ion battery electrodes, where micron-scale particles are held together by a conductive polymeric binder and surrounded by electrolyte. The morphology of the particle and conductive binder structures greatly affect macroscale properties and can vary significantly as a function of manufacturing conditions. While it is possible to image these mesostructures using x-ray computed tomography (XCT), subsequent meshing and finite element analysis often proves challenging and time consuming.

In this talk we apply the Conformal Decomposition Finite Element Method (CDFEM) as a rapid meshing and analysis technique for calculating effective properties such as thermal conductivity, electrical conductivity, tortuosity, permeability, and mechanical modulus of battery electrode materials. Mesostructures are obtained via two methods. First, 3D XCT images are processed and individual particles identified. Second, a discrete element method (DEM) simulation is performed to recreate mesostructures that replicate the image data, but in a more rapid and parameterized fashion. The results of these two approaches are compared. We quantify how CDFEM can be used to rapidly and reproducibly obtain computable meshes on complex geometries and can be a tool for rapid turnaround analysis.

Title: Reimagining the CAE Workflow Via Polyhedral Finite Elements

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Abstract: This talk seeks to address how rapid design-to-analysis might be conceptualized most usefully from the perspective of the user-engineer. Some of the central questions: can the solid-modeling part of the workflow be configured so that the subsequent analysis phase is made easier for the engineer? What is the optimal point in the workflow for the introduction of the mesh or other spatial discretization? Are there benefits to assigning BVP-related attributes, such as material models, boundary conditions, and volumetric loading, to the solid model itself, in advance of domain discretization? What is the most useful format for specifying the desired level of discretization refinement and its spatial distribution? In the talk, specific answers to these questions are posited, animated by the Partitioned Element Method (PEM). The PEM is an instance of the class of polyhedral finite element methods, all of which share certain finite-element-like attributes: displacement-based Galerkin approximation of the weak problem statement, discretization of the problem domain into disjoint elements, and quadrature domains that align with the basis-function supports, among other things. The PEM is based on a partition of each element into cells. The cell complex facilitates both formulation of the element's quadrature rule, as well as synthesis of the discrete shape functions. Brief accounts of the PEM element formulation, and of a PEM-based Computer-Aided Engineering workflow, will be given.

Title: The Conforming Reproducing Kernel Method for an Agile Design-to-Simulation Workflow

Presenter: Jacob Koester
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Additional Co-Author(s): Mitchell, Scott; Sandia National Laboratories Bishop, Joseph; Sandia National Laboratories

Abstract: Efficient model development for complex systems remains a challenge. Generating a mesh of sufficient quality for the Finite Element Method (FEM) can take months [1]. Research in agile design-to-simulation processes seeks to alleviate this bottleneck by taking on the difficult task of pairing automatic discretization techniques with numerical methods that are capable of producing satisfactory results. In this work, we present the Conforming Reproducing Kernel (CRK) numerical method. In this new approach, approximation functions are constructed using the reproducing kernel method with kernel functions created using Bernstein-Bezier splines on local geometry subdivisions. Meshfree methods, such as the Reproducing Kernel Particle Method (RKPM) [2], have an advantage over FEM as a high-quality mesh is not required. However, this flexibility in the construction of shape functions does present new challenges. Domain integration must be reformulated in order to maintain high accuracy and efficiency [3]. Concave geometries require special consideration so concavities are preserved. Material interfaces call for special attention so that weak discontinuities can be captured. Also, the underlying reproducing kernel method gives CRK the flexibility to blend approximations over low quality subdivisions or handle non-contiguous meshes, making it compatible with automatic discretization processes that produce may produce low quality meshes. Previous work focused on developing the concept in two dimensions using C1 splines on triangulations. In this presentation, the method is extended to three dimensions and kernels are constructed using tetrahedral subdivisions. Examples utilizing the conforming kernels are shown and results are compared to predictions using FEM and RKPM. REFERENCES [1] M. Hardwick, R. Clay, P. Boggs, E. Walsh, A. Larzelere and A. Altshuler, DART system analysis, SAND2005-4647, Sandia National Laboratories, Albuquerque, NM, 2005. [2] W.K. Liu, S. Jun and Y.F. Zhang, Reproducing kernel particle methods, International Journal for Numerical Methods in Fluids, 20, 1081-1106, 1995. [3] J.S. Chen, M. Hillman and M. Rüter, An arbitrary order variationally consistent integration for Galerkin meshfree methods, International Journal for Numerical Methods in Engineering, 95, 387-418, 2013. *Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for

the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Title: VoroCrust: Conforming Voronoi meshing of non-convex domains with sharp features and narrow regions

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Abstract: We present VoroCrust: a novel approach to polyhedral meshing that simultaneously generates a quality mesh of the surface of a Piecewise Linear Complex (PLC) model and decomposes the enclosed volume by unweighted Voronoi cells with good aspect ratios conforming to the surface mesh, without clipping or bad normals. VoroCrust has an embedded sizing function that capture the curvature of the model, and robustly represents sharp features and narrow regions that may be associated with the input model. Up to our knowledge, VoroCrust is the first to solve this open problem. VoroCrust also outputs an approximation of the medial axis of the input model and provides a fast technique for in/out point classification. A variation of VoroCrust can also handle non-manifold and non-watertight inputs. We illustrate the robustness and output quality of VoroCrust through a collection of models of varying complexity. In this talk we also present the recently released VoroCrust software and discuss its performance in practice. VoroCrust generates non-clipped Voronoi cells everywhere, and hence the generated Voronoi seeds underlying defines the underlying mesh eliminating the need to generate the entities of the explicit mesh.

6 Penetration and Perforation

Title: Optimal Transportation Meshfree Simulation of Whipple Shield under Hypervelocity Impact

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Abstract: Space debris hypervelocity impact (HVI) poses a serious threat to the safety of space vehicles. For debris smaller than 1 cm in size, Whipple shield is the major means of protection. Large scale three-dimensional numerical simulations of HVI of Aluminum alloy 6061-T6 plates by the same material sphere projectile have been performed using the Optimal Transportation Meshfree (OTM) method, along with the seizing contact and variational material point failure algorithm. The dynamic response of the Al6061-T6 plate including phase transition in the high strain rate, high pressure and high temperature regime expected in our numerical analysis is described by the use of a variational thermomechanical coupling constitutive model with SESAME equation of state, rate-dependent J2 plasticity with power law hardening and thermal softening and temperature dependent Newtonian viscosity. The evaluation of the performance of the numerical model takes the form of a conventional validation analysis. In support of the analysis, we have compared OTM results with the experiments in literature over a range of impact velocities of 4.47 6.15km/s, a range of projectile diameters of 4mm and 5mm, and a range of obliquities of 0° and 45°. Large scale three-dimensional OTM simulations of HVI are performed on departmental class systems using a dynamic load balancing MPI/PThreads parallel implementation of the OTM method. We find excellent full field agreement between measured and computed perforation size, and debris cloud.

Title: A Multiscale Model for Sand

Presenter: David Littlefield
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Abstract: In recent years, renewed research effort has been directed toward characterizing soils in transient applications. The main approach favored towards that end, has been to use one of many "cap" models derived from Mohr-Coulomb failure theory. In addition to a friction-based yielding stress like Mohr-Coulomb, typically such models incorporate a pressure cap. More advanced three-phase models also take into account the great difference in soil response with degree of saturation through "effective" stress. Effective stress isolates the stress in the solid skeleton of the material, from the bulk behavior. One such model, the Hybrid Elastic Plastic (HEP) model has been used extensively to model soils subjected to energetic, highly-transient phenomena using hydrocodes, a class of explicit computational packages geared toward such phenomena.

Geomaterials such as soils, differ from other common engineering materials like metals, polymers, and many composites, in that the fundamental evolution of the underlying structure may reasonably be considered to occur at a higher scale, i.e. at the mesoscale rather than the microscale. This offers a somewhat unique opportunity to be able to characterize the underlying structural evolution of the material, and use that characterization to inform a general constitutive framework to model the behavior of a wide spectrum of soils under a range of pressures and distortional transient loading conditions.

In the current work, experimental and laboratory data of a poorly graded sand previously modeled using the HEP model, is used to explore the internal evolution of the sand by carrying out particle-based simulations of the behavior at the mesoscale. These simulations are used to conduct a homogenization study of the granular subdomain. This is done in order to 1) identify the threshold at which the transition from discrete mesoscale to the Representative Volume Element (RVE) occurs, and 2) to quantify the uncertainty associated with discretization below that threshold. Additionally, the mesoscale results are used to formulate an effective stress model that matches the behavior observed in the particle-based simulations. This new effective stress model is then compared with the predictions of the sand behavior from the HEP model.

Title: Modeling Penetration and Perforation with Peridynamics

Presenter: Stewart Silling
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Abstract: The peridynamic theory simulates the nucleation and growth of multiple, mutually interacting, dynamic fractures. This capability makes it a natural candidate for modeling impact problems involving fragmentation and other aspects of high-rate material failure. This talk will describe the theory and its meshless implementation. Numerical examples demonstrate the capabilities of the method for impact and penetration applications over a range of velocities and target properties.

Title: Reproducing Kernel Particle Method Modeling of Ultra-High Performance Concrete Flyer Plate Experiments

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Abstract: Ultra-high performance concrete (UHPC) has emerged as a viable material in protective structures of interest to the defense community. One area that has little study is under extreme loading conditions such as high velocity flyer plate impacts that induce shock wave propagation. Some recent work by Neel et al. [3] produced a number of carefully controlled flyer plate impact experiments for a UHPC. This data provides an excellent testbed to evaluate some current computational solid mechanics codes and their respective constitutive model's ability to model this extreme loading condition. The data from Neel et al. [1] can be used to calibrate and validate a computational methods ability to match this type of loading condition. This study investigates modeling the flyer plate experiments of Neel et al. [1] using the meshfree method known as the reproducing kernel particle method (RKPM). Recent work by Roth et al. [2] and Zhou [3] has shown shock waves can be modeled in an RKPM framework. RKPM coupled with the advanced fundamental concrete model will be used to model the flyer plate experiments. The RKPM approach will also be applied to a simple penetration problem in order to quantify the effect of including the corrected shock behavior. A discussion of the different current strengths and weaknesses of the RKPM approach will be discussed as well as some future recommended research areas.

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Title: Particle Conversion Methods for Computing Momentum Enhancement due to Hyper-velocity Impact

Presenter: James D. Walker
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Abstract: Hypervelocity impacts (> 2 km/s) typically lead to large craters and the liberation of material from the target, referred to as ejecta. The ejecta leave the impact site at a variety of velocities. Momentum enhancement is the effect that the crater ejecta lead to more momentum being transferred to the target than solely the momentum of the projectile. Experimentally the effect can be relatively large, i.e., doubling the momentum delivered to the target, and more. Computing the momentum enhancement in a large scale numerical simulation is a challenge. It relies on accurate calculation of the failure (separation) of material in the crater during crater formation and then the throwing off of the failed material in the opposite direction at the correct speed. A common approach in Lagrangian finite element computations of penetration events is to have an erosion criterion so that elements are discarded when they are highly distorted and invert or otherwise adversely affect the time step. However, to compute momentum enhancement, it is not possible to discard material. Thus, we have been using the particle conversion routines in the EPIC hydrocode to study momentum enhancement. This feature converts a finite element that reaches a failure threshold to a particle, thus conserving mass. The particle interacts with other particles and with the remaining finite element mesh to conserve momentum. This talk will present numerical studies with comparisons to experiments performed at Southwest Research Institute. The experiments are impacts of aluminum spheres of 2.54 and 4.45 cm in diameter at speeds slightly above 2 km/s into various geological materials, including granite and pumice. The role of the particle conversion as well as the constitutive model in the numerical simulations will be discussed. There will also be comparisons of the EPIC results using particle conversion with Eulerian computations with the hydrocode CTH.

7 Damage and Fracture

Title: A Partition of Unity Method for Thermal Hydraulic Fracturing

Presenter: Albert Ziegenhagel
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Abstract: Hydraulic fracturing is subject to many different physical phenomena. These include the deformation of the surrounding rock, the fluid flow within the fracture and leak-off of the fracking fluid into the permeable rock. Additionally, thermal effects of the fluid as well as of the surrounding rock can influence the behavior of the whole system and especially the crack propagation.

The simulation of the propagation of hydraulic fractures under those conditions puts many challenges on the numerical methods used. We present an implementation via the framework PUMA [1] based on a flat-top partition of unity method (PUM) [2] to discretize and solve the mixed, non-linear system of equations that are implied by this problem.

We present a novel approach to the governing equations for the thermal hydraulic fracturing process together with numerical results that show how the involved temperature can influence the propagation of the crack.

[1] Fraunhofer SCAI - PUMA, https://www.scai.fraunhofer.de/en/business-research-areas/meshfree-multiscale-methods/products/puma.html

[2] M. A. Schweitzer, A Parallel Multilevel Partition of Unity Method for Elliptic Partial Differential Equations, Lecture Notes in Computational Science and Engineering, 29, 2003

Title: Peridynamic modeling of dynamic fracture in metallic materials

Presenter: Masoud Behzadinasab
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Abstract: Prediction of crack initiation, propagation, and ductile fracture can be very challenging in metallic materials with complex geometries. Damage accumulation along the plastic loading path governs the fracture initiation in ductile materials. Over the past two decades, the peridynamic theory has been exploited for modeling dynamic problems involving fracture. Peridynamics has, however, mostly applied in modeling fracture in brittle materials, and its robustness in ductile fracture modeling has not been fully explored. Recently Foster et al. (2017) proposed a new framework to incorporate classical finite deformation material models in peridynamics. Tupek et al. (2013) has also introduced a constitutive damage modeling approach for peridyanmics to take advantage of the well-established classical damage models. A material model corresponding to the finite strain elastoplasticity theory of Simo (1988) and a damage model corresponding to Johnson-Cook model (1985) have been implemented in Peridigm, an open-source massively-parallel computational peridynamics code. This framework has been applied to the Sandia Fracture Challenge 3. The model was first calibrated by the data provided by Sandia National Laboratories. Following that, a blind prediction was performed on the challenge geometry and results were compared.

Title: Micromechanical Studies of Compressive Strength in Brittle Polycrystalline Materials at High Strain Rates

Presenter: Bo Li
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Abstract: We propose a micromechanical computational framework for the high fidelity prediction of failure mechanisms in brittle polycrystalline materials. A three-dimensional direct numerical simulation of polycrystalline structures is constructed to explicitly account for the microstructural features, such as grain sizes, grain orientations, and grain boundary misorientations, by using the Optimal Transportation Meshfree (OTM) method. In particular, grain boundaries are represented by a thin layer of material points with nonzero misorientation angles. The EigenErosion algorithm is employed to predict the crack propagation in the grain structure including intergranular and transgranular fractures. In the EigenErosion approach, an equivalent energy release rate is defined at the material points to evaluate the local failure state by comparing to the critical energy release rate, which varies at the grain boundaries and the interior of grains. Moreover, the constitutive model is considered as functions of the local microstructure features. As a result, the anisotropic response of brittle polycrystalline materials and the interaction between the fracture and topological defects in the microstructure under general loading conditions can be explicitly modeled. Finally, the compressive dynamic response of hexagonal SiC with equiaxed grain structures is studied at different strain rates by using the proposed computational framework. The predicted strain rate dependence in the compressive strength of SiC agrees well with measurements in Split Hopkins Pressure Bar (SHPB) experiments. A micromechanics-based interpretation for the strain rate dependent fracture properties in brittle materials is derived by quantifying the competition and combination of intergranular and transgranular fractures in the polycrystalline structures.

8 Advanced Manufacturing

Title: Integrating Nonlocal Constitutive Modeling with Nonlocal MPM for Better Evaluating Multi-Physical Responses

Presenter: Zhen Chen
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Abstract: Multi-phase (solid-liquid-gas or soft-hard material interfacial) interactions play an important role in modern engineering applications such as additive manufacturing, drilling, hydrofracturing, impact and penetration. It has been shown that the evolution of interfacial failure between different material phases has the nonlocal feature [Chen and Schreyer,1994; among others], namely, the stress state at a material point depends on the strain distribution around that point in a representative volume of certain size. Hence, local constitutive models cannot predict the real physics associated with interfacial failure evolution. On the other hand, the mesh-based methods cannot describe the real physics involved in the interfacial problems, due to the use of master/slave nodes at the contact surface of (assumed) zero thickness in addition to re-meshing as required for the simulation of failure evolution. To better simulate the multi-phase interactions, the material point method (MPM) has evolved over the last two and a half decades, and been applied to many areas of Simulation-based Engineering Science, as shown in the recent comprehensive review [Zhang et al., 2016]. To improve the solution accuracy for large deformation cases, very recent efforts have been made to enhance the MPM with B-spline basis functions [Gan et al., 2018], and time-discontinuous mapping operation [Lu et al., 2018]. Based on the conservation laws of mass, momentum and energy, the generalized interpolation material point (GIMP) method has also been improved for simulating and evaluating the fully coupled thermomechanical responses, such as the failure evolution in a snowy slope [Tao et al., 2018]. Since the improvement over the original MPM is essentially to replace the local mapping and remapping process with a nonlocal one at additional computational costs, it might be feasible for us to integrate nonlocal constitutive modeling with the smoothed operator for efficient model-based simulation. In the workshop, an effort will be made to explore the way to do so, with a focus on the multi-physics involved in multi-phase interactions.

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Title: Numerical modeling of the hot forming process of composite materials

Presenter: Hao Wang
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Abstract: We present a fully coupled thermomechanical simulation of the hot forming process of composite materials. The hot forming process consists of several loading cycles, and each cycle has three steps: hot compression, steady heat conduction and relaxation. The raw material is composed of matrix powders with resin, strengthening particles and reinforcing fibers. The compression ratio of the material during the fabrication process can reach as high as 80This proposed method combines the Optimal Transportation Meshfree (OTM) method and the variational thermomechanical constitutive updates. The variational structure of dynamic systems with general internal dissipative mechanisms is discretized in time by applying the Optimal Transportation theory. Furthermore, material points and nodes are introduced for the spatial discretization of the domain. In addition, kinematic information of the system including displacement and temperature is defined at the nodes, while material local state and constitutive responses are evaluated at the material points. Meanwhile, the Local Maximum Entropy (LME) approximation method is introduced as shape function to construct the continuous incremental motion and temperature field. The deformation, temperature and internal variables are therefore obtained at the stationary of the fully discretized action. An operator splitting algorithm is adopted in the simulation. Specifically, at each iteration, the discretized mechanical equations are solved explicitly at the nodes with embedded implicit processes to compute the internal variables at material points assuming adiabatic conditions. The discretized thermal equations are then solved implicitly assuming mechanical equilibrium to update the temperature field. Assuming the deformation and temperature are fixed, the curing degree of the matrix is calculated by using an empirical curing model. Finally, the gas transportation in the porous matrix is calculated by Darcy's law. The computational framework is validated by comparing the predicted compression ratio, material properties, reorientation of fibers and void volume fraction to the experimental measurements. It enables a robust and efficient analysis for the sensitivity of the properties of composite materials on their processing parameters.

Title: Direct Numerical Simulation of Powder Bed Fusion Based Additive Manufacturing of Metals

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Abstract: Powder bed fusion (PBF) based additive manufacturing technology is one of the most widely used techniques of all additive manufacturing (AM) techniques for the fabrication of metallic components. The goals of our research are to develop a powder-scale direct numerical simulation (DNS) capability for the PBF processes based on the novel Hot Optimal Transportation Meshfree (HOTM) method and to discover the process parameters-microstructure-material properties-component performance relationship for PBF AM process through DNS. The HOTM method is a meshfree thermomechanical Lagrangian computational framework for materials behaviors under extreme thermomechanical loading conditions, which combines the Optimal Transportation Meshfree (OTM) method and the variational thermomechanical constitutive updates. Material points and nodes are introduced for the spatial discretization of the domain. At each iteration, the discretized mechanical equations are solved explicitly at the nodes with embedded implicit processes to compute the internal variables at material points assuming adiabatic conditions. The discretized thermal equations are then solved implicitly assuming mechanical equilibrium to update the temperature distribution. A phase-aware constitutive model is developed to simulate the phase change (e.g., melting, vaporization and solidification) and multiphase mixing of the PBF AM process automatically, where the temperature directly determines the material local state. A method to model realistic powder bed geometry based on the statistic information measured from experiments (such as a powder bed particle size and shape distribution, packing density, powder quality, and thermomechanical properties of individual particles, etc.) is developed. A recoil pressure model and a surface tension model in the Lagrangian framework are developed to directly simulate the melt pool dynamics and the Marangoni effect. Different heat flux models are developed to represent various power beams with different characteristics, such as power level, size, and absorptivity, scan speed and path. The convective heat flux model and radiation heat flux model between the powder bed and the environment are also developed within our model. The influence of different powers and speeds of the laser heat flux on the melting of the powder bed is studied by the DNS of the PBF process for a multi-layer powder bed.

Title: Smoothed Particle Galerkin Method with a Momentum-Consistent Smoothing Algorithm for Explicit Coupled Thermal-Structural Analysis

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Abstract: This paper introduces a momentum-consistent smoothing algorithm to Smoothed Particle Galerkin (SPG) method in LS-DYNA for the explicit coupled thermal-structural analysis. In contrast to the kernel approximation in conventional Lagrangian particle methods, the system of equations of the present method is discretized and approximated following that in the SPG method. The momentum-consistently smoothing algorithm provides the desired stability and accuracy in the thermal structural coupling applications. Furthermore, the algorithm is coupled with FEM with sharing nodes to increase the computational efficiency. Two benchmarks including heat flux and thermal expansion are studied to demonstrate the accuracy of the present method. In addition, the frictional drilling test is simulated to demonstrate the effectiveness of the proposed method in the coupled thermal-structural analysis involving material failure.

Title: Discrete element modeling of powder spreading for metal additive manufacturing

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Abstract: Metal additive manufacturing technologies such as selective laser melting rely on layer-by-layer deposition of powder. The structure of the resulting powder bed is not readily accessible to experiments, but it likely affects the formation of defects in the manufactured part. This motivates a modeling study that connects powder feedstock properties, spreading process parameters and powder bed characteristics. In many cases, relevant process length scales (e.g. powder layer thickness, laser spot size) are comparable to the length scale of individual particles, which obviates the use of continuum models of powder deposition. We therefore employ the discrete element method (DEM) to simulate the powder deposition process, which resolves the dynamics of individual powder particles. DEM simulations can account for arbitrary variations in particle-scale properties such as particle size and shape distribution, as well as various aspects of interparticle contact mechanics, such as variations in friction (e.g. due to particle surface roughness) or variations in interparticle cohesion (e.g. due to chemical composition and particle surface morphology). In order to capture these effects, we employ relatively complex contact models that include multiple modes of history-dependent friction (sliding, rolling and twisting modes) as well as viscoelastic and cohesive forces. We present a systematic sensitivity analysis that relates variations in these contact parameters to relevant structural metrics of the resulting powder bed. We show that both interparticle friction and cohesion have a significant effect on powder bed structure. Furthermore, we describe a framework for calibrating and validating DEM models in the context of powder rheology, which offers a systematic connection between particle-scale micromechanical parameters and experimentally accessible bulk flow measures.

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9 Fluid-Structure Interactions and Other Coupled Problems

Title: A monolithic Lagrangian meshfree method for Fluid-Structure Interaction problems within the OTM framework

Presenter: Renjie Ke
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Abstract: We present a monolithic Lagrangian meshfree solution for Fluid-Structure Interaction (FSI) problems within the Optimal Transportation Meshfree (OTM) framework. A uniform set of governing equations are formulated in the Lagrangian configuration and solved simultaneously in a monolithic way. In this framework, the fluid-structure interface becomes an internal surface of the entire field, and the continuity and force equilibrium on the interface are automatically satisfied without extra treatments leading to a more stable and accurate solution with fast convergence. The monolithic Lagrangian solution eliminates the problem of free surface and material interface tracking in contrast to the partitioning approaches. The presented method enables a Direct Numerical Simulation (DNS) of the fluid flow with the absence of the convective terms. Meanwhile, a MPI/Multithreads hybrid parallelization of OTM method is also enabled in simulations. We illustrate the ability of our numerical framework to simulate the fluid interaction with highly flexible structures through two examples: the deformation and adhesion of single human Red Blood Cell (RBC) in a microchannel and tumor cell dynamics in a micro-device. The presented method is employed to simulate the experimental configuration directly. For RBC simulation, we model the RBC as a membrane enclosing a nearly incompressible Cytoplasm such that cell deformation is a complex procedure involving with membrane-Cytoplasm, membrane-plasma interactions, and is also determined by the membrane mechanical properties as well as endothelium contact conditions. The mechanical properties of cell membrane can be calibrated from the simulation results of geometric deformation comparing to the experimental observations. The cellular adhesion is simulated by using a multiscale constitutive model at continuum level to predict the viscoelastic response of ligand-receptor bonds. For tumor simulation, we simulate two tumor cell deformation and motion in the streaming flow generated by resonant device. Tumor cell is modeled the same way as RBC, moreover, the physical contact is defined directly using OTM contact algorithm for modeling the tumor cell-cell interaction. In summary, the OTM FSI approach can be used to study the cell-fluid interaction, cell-cell interaction, cell deformation, adhesion and separation, which enables quantitative determination of the underlying cell mechanism in various flow conditions.

Title: Peridynamic contact modeling in i(mmer)sogeometric analysis

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Abstract: We describe a hybrid peridynamic–isogeometric approach to analyzing complicated contact problems. Our approach uses a peridynamic model and meshfree discretization of contact, coupled to an isogeometric discretization of the structure's (local) continuum mechanics. The peridynamic formulation can be viewed as a continuous model corresponding to a variant of the discrete "pinball algorithm" proposed by Belytschko and collaborators several decades ago. We demonstrate the algorithmic simplicity of the method by reviewing a remarkably-concise implementation of nontrivial contact between Kirchhoff–Love shell structures. This implementation is only a few hundred lines of Python code and uses our recent open-source isogeometric analysis library tIGAr, which leverages finite element automation technology from the FEniCS project. We demonstrate the robustness of our peridynamic–isogeometric contact approach by applying it within simulations of natural and artificial heart valves, including immersogeometric fluid–structure interaction analysis.

Title: Recent Advances in IGA-Meshfree Coupling for Air-Blast FSI

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Abstract: A novel framework for air-blast-structure interaction (ABSI) based on an immersed approach coupling IGA and RKPM-based Meshfree methods is presented and verified on a set of challenging problems. A novel Phase-Field methodology for brittle fracture, amenable to explicit time integration, is presented. Its coupling with the ABSI framework is also presented, and the coupled framework is deployed on a set of challenging examples.

10 Shock and Hydrodynamics

Title: A Lagrangian Gradient Smoothing Method (L-GSM) Model for free surface flows

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Abstract: A novel Lagrangian gradient smoothing (L-GSM) model for free surface flows will be presented. This consists of the following six parts: 1) a conservatively discretized GSM form of differential governing equations; 2) an exclusive nearest neighboring particles searching (NNPS) algorithm for L-GSM simulation; 3) an unconditionally consistent GSM technique to approximate the gradients of variables in the differential governing equations; 4) an artificial velocity for L-GSM particles marching; 5) Four applications to validate this new numerical model: dam break with an obstacle, dam break with multiple wall impacts, water discharge from a container and water splash; 6) advantages and disadvantages of the L-GSM method and its future development.

This study highly depends on the works in [1] and [2], where [1] first extended the Eulerian gradient smoothing method [3] to Lagrangian system, and comprehensively studied the accuracy, stability condition and the computational efficiency of L-GSM method, and [2] is a comparative SPH model for free surface flows that is used to validate the L-GSM solutions. As widely known, the advantage of Lagrangian meshfree methods over the traditional grid-based methods is its much better performance in extremely large deformation problems simulation, like explosion, penetration and free surface flows. This study aims to extending our previous L-GSM model in [1] to free surface flows simulation by developing some techniques as shown in parts 1)-4) in the first paragraph.

This work will provide an alternative to free surface flows simulation which owns typically the same accuracy condition as SPH but a much better efficiency in computation. Moreover, as demonstrated and evidenced in [1], the L-GSM model does not suffer from the tensile instability problem that widely existing in SPH simulation. References: [1] Mao Z, Liu GR. A Lagrangian gradient smoothing method for solid-flow problems using simplicial mesh. Int J Numer Methods Eng. 2018; 113:858–890. [2] J. J. Monaghan, Simulating Free Surface Flows with SPH, J. Comput. Phys. 1994; 110(2): 399–406. [3] G. R. Liu and G. X. Xu, “A gradient smoothing method (GSM) for fluid dynamics problems,” Int. J. Numer. Methods Fluids, 2008; 58(10): 1101–1133.

Title: Eulerian Reproducing Kernel Particle Method for Shock Modeling

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Abstract: The following issues need to be properly addressed in modeling shock wave propagation in hydrodynamical systems: (1) correct representation of essential shock physics, (2) stabilization of Gibbs phenomenon at discontinuity, and (3) capturing shock front with minimal smearing of moving discontinuity. In this work, we introduce a stabilized Eulerian reproducing kernel particle method (RKPM) for shock modeling. RKPM is considered herein due to its versatility in adaptive refinement and in adjusting smoothness independently to the order of completeness in the approximation. A smoothed flex is constructed with local Riemann-enrichment, such that the essential shock physics are satisfied. The oscillation control is provided through the smoothed flux divergence. Flux vector splitting approach is employed for the stabilization of advection in shock modeling. A Monotonic Upstream-Centered Scheme for Conservation Laws (MUSCL) type flux reconstruction with oscillation limiter is introduced for higher order spatial accuracy. Several numerical examples are analyzed to verify the effectiveness of the proposed framework.

Title: Generalized Anisotropic Gruneisen Parameter: A Vector Equation of State for Anisotropic Materials

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Abstract: During moderate to high levels of shock loading, the material undergoes nonlinear behavior in which the deformation is thermodynamically coupled with the internal energy; therefore, an equation of state (EOS) is required to describe the material's response to these conditions. This problem has been satisfactory addressed in the isotropic solid-state physics and mechanics problems. In recent years, numerous investigations into the mechanical properties of different classes of anisotropic materials under shock loading conditions have been undertaken. However, despite a perfectly adequate general understanding, experimental methodology, and theory, there are no unified anisotropic EOS models. Using the concept of the generalized decomposition of the stress tensor (Lukyanov, 2008), the modified definition of the generalized bulk Gruneisen parameters and associated anisotropic EOS in the parametric space of generalized decompositions are derived in a vector form and presented in this paper. The thermomechanical generalized Gruneisen parameter has been define as the generalized thermodynamic pressure response in a material to a change in internal energy with the strains held constant which considers for the oriented response of anisotropic materials. The behavior of aluminum alloy 7010-T6 under shock loading conditions using plate- and Taylor- impact tests are modelled using meshless methods. A comparison of numerical simulations with existing experimental data shows good agreement of the general pulse shape, Hugoniot Elastic Limits (HELs), and Hugoniot stress levels, and suggests that the proposed unified anisotropic EOS, strength models and meshless numerical method are performing satisfactorily.

Title: Adaptive reconnection-based Arbitrary Lagrangian Eulerian method - A-ReALE

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Abstract: We present a new adaptive reconnection-based Arbitrary Lagrangian Eulerian method - A-ReALE. The main elements of an A-ReALE method 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 - both number of cells and their locations as well as connectivity (based on using Voronoi tessellation) of the mesh are allowed to change; and a remapping phase in which the Lagrangian solution is transferred onto the new grid. The design principles of A-ReALE method can be summarized as follows. 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 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. 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.

Title: Coupled Shock-Plasticity-Damage Modeling of Explosive Welding by RKPM

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Abstract: The explosive welding (EXW) process entails shock waves, large plastic deformation, and fragmentation around the collision point, troubling the traditional mesh-based methods for reliable solution. In this work, a computational framework based on the semi-Lagrangian reproducing kernel particle method (SL-RKPM) [1] is introduced for the modeling of EXW. For modeling shocks in plastically deformed solid, a Godunov-type shock algorithm formulated under the stabilized non-conforming nodal integration (SNNI) framework [2] is employed, where the Godunov scheme is embedded in the volumetric strain energy via a purely node-based flux gradient evaluation which ensures the linear momentum conservation. The Gibbs instability is controlled through the smoothed flux divergence in SNNI. The effects of high strain-rate and high temperature on plasticity and damage in the metals are taken into consideration in the material law. A strain-rate-dependent update of kernel supports and strain smoothing cells for SNNI is introduced to accurately capture excessive plastic flow and metal jetting. Adaptive refinement strategies near the contact interface are also introduced. The kinematics of the flyer plate, jet formation, smooth to wavy interface morphologies transition, and the welding condition along the metal interface are compared to several experimental results to validate the effectiveness of the proposed methods for EXW modeling.

References [1] Guan, P., Chen, J.S., Wu, Y., Teng, H., Gaidos, J., Hofstetter, K., Alsaleh, M. Semi-Lagrangian reproducing kernel formulation and application to modeling earth moving operations. Mechanics of Materials 2009; 41(6):670–683. [2] Zhou, G., Chen, J.S., and Hillman, M. A Godunov-type Semi-Lagrangian Galerkin Meshfree Method for Modeling Shocks in Solid and Fluid, to be submitted.

11 Geoscience and Natural Disasters

Title: Reduction of numerical errors in material point method

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Abstract: The material point method (MPM) is a continuum-based particle method frequently used for complex geotechnical problems. MPM can be viewed as an extension of the finite element method (FEM) that combines Lagrangian and Eulerian frames to successfully avoid numerical diffusion associated with the convective terms in the Eulerian approach and prevent mesh distortion due to large deformations observed with the Lagrangian approach. Despite this, MPM still contains many numerical shortcomings. First of all, MPM projects the material-point data to the background mesh and vice versa using piecewise-linear basis functions. The discontinuous gradients of these basis functions lead to unphysical oscillations in the solution when particles cross element boundaries. In addition, the method reconstructs scattered material-point data using a low-order function-reconstruction technique that causes severe inaccuracies when large deformations are involved. Finally, MPM inherits the shortcomings of the FEM such as errors due to time-integration and lumping of the mass matrix. In this talk, we present possible numerical improvements for the standard MPM scheme. Similarly to piecewise-linear basis functions, higher-order B-spline basis functions feature mathematical properties valuable for MPM (e.g., partition of unity). However, they have an important advantage: smooth gradients of higher-order B-splines significantly reduce the grid crossing errors. We attempt to bridge the gap in terms of the complexity between the B-spline basis functions and piecewise-linear basis functions, by using the recursive Cox-de Boor formula. A further improvement of the spatial accuracy is achieved by the Taylor Least Squares (TLS) reconstruction technique, a local least-squares approximation obtained with the polynomial Taylor basis. In contrast to other advanced reconstruction techniques, the TLS approach preserves the total mass and linear momentum after the reconstruction. Furthermore, in combination with an exact quadrature rule, TLS guarantees the conservation of mass and momentum during the transfer of information from material points to the grid. While the spatial errors are dominating in MPM, a fully higher-order method cannot be obtained without adjusting the time-integration scheme. Replacing Euler-Cromer method adopted in the standard MPM by higher-order Runge-Kutta methods offers such possibility.

Title: A Meshfree Computational Framework for Modeling Hydro-Mechanical Damage Processes in Porous Geomaterials

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Abstract: In this work, a stabilized RKPM (Reproducing Kernel Particle Method) formulation for hydro-mechanical modeling of multiphase porous media is developed. Under the variationally consistent nodal integration framework [1], the fluid pressure projection method is introduced to achieve a stable equal-order u-p reproducing kernel approximation for the mixed formulation [2]. It is shown that the present approach can effectively eliminate the nodal integration-induced spurious low-energy modes, as well as non-physical fluid pressure oscillations due to the violation of inf-sup condition. To capture complex evolving crack patterns in porous geo-materials, the damage particle method [3] which approximates fractures by a set of damaged particles is introduced under the RKPM discretization. For each damaged particle, a regularized smeared description of the equivalent crack segment at the nodal position is adopted, which avoids spurious mesh dependency issues in conventional methods. The proposed computational framework is applied to the modeling of landslide and hydraulic fracturing processes.

References [1] Chen, J.S., Hillman, M., Rüter, M. (2013) An arbitrary order variationally consistent integration method for Galerkin meshfree methods. International Journal for Numerical Methods in Engineering, 95(5): 387-418. [2] Wei, H., Chen, J.S., & Hillman, M. (2016). A stabilized nodally integrated meshfree formulation for fully coupled hydro-mechanical analysis of fluid-saturated porous media. Computers & Fluids, 141, 105-115. [3] Wei, H, Chen, J.S. (2018). A damage particle method for smeared modeling of brittle fracture. International Journal for Multiscale Computational Engineering, DOI: 10.1615/IntJMultCompEng.2018026133.

Title: 1D MPM-DEM Hierarchical Multiscale Modeling of a Split Hopkinson Pressure Bar Experiment on Dry Colorado Mason Sand

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Abstract: In an effort to strike balance between the fidelity of direct numerical simulations and the computational efficiency of continuum models of soils, a hierarchical multiscale model was developed to model the large strain, high strain rate split Hopkinson pressure bar experiments conducted on dry Colorado Mason sand. A one-dimensional implementation of the material point method (MPM) was used to model the geometry of the experiment, and rather than developing a phenomenological constitutive model for the dry sand, ellipsoidal discrete element method (DEM) particle assemblies were generated from synchrotron microcomputed tomography imaging of the the soil and used in place of the constitutive model in the continuum method. MPM calculated the deformation gradient over the domain by solving the momentum equation, which was then passed as boundary conditions to the DEM assemblies. After deforming, a homogenized Cauchy stress over the DEM assemblies was passed back to the continuum models. The MPM-DEM model was then verified against and compared to a similar FEM-DEM hierarchical multiscale model. Three different versions of the MPM-DEM model representing differing background grid and material point densities over the problem geometry were then run to evaluate the effect of the material point method on the hierarchical multiscale algorithm. Results from the simulations show the ability to reasonably reproduce the experimental results and compared favorably with the FEM-DEM simulation results. Although more modern MPM basis functions will need to be implemented, the MPM-DEM model shows promise in modeling large deformation, high strain rate problems.

Title: A Discrete Element Model for Sea Ice

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Abstract: Sea ice is an important component of the global climate system, reflecting a significant amount of solar radiation, insulating the ocean from the atmosphere and influencing ocean circulation by modifying the salinity of the upper ocean. Sea ice is composed of rigid plates called floes that are transported due to winds and ocean currents. Interacting floes can separate forming regions of open water or converge creating large ice ridges. Most sea ice models used today for global or large regional simulations rely on a continuum approximation for the ice cover. However, the models are often run at high grid resolutions (5-10 km), which are beyond the point where the continuum approximation breaks down and the interactions between floes dominate the dynamics.

To address this deficiency, we are developing a new sea ice dynamical core based on the Discrete Element Method (DEM) where collections of floes are explicitly modeled as discrete elements that interact through contact forces. With this method, no averaging to produce a continuum is performed, and the brittle, highly heterogeneous and anisotropic nature of the ice pack can be captured. In this talk we will describe the initial implementation of our DEM model, which is built upon the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code. Utilizing LAMMPS for the DEM dynamics provides a high-performance core and enables the use of the Kokkos programming model for porting to heterogeneous architectures. We have implemented an element contact force model suitable for sea ice that allows elements to freeze together and fracture apart and incorporated radiative effects through a coupled column thermodynamics model. Test cases will be shown to illustrate the implementation and future goals for the model will be addressed.

12 Implementation and High-Performance Computing

Title: Meshless Transfer for Earth System Models via the Compadre Toolkit

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Abstract: We will be introducing users to the Compadre Toolkit as it relates to the coupling of Global Earth System Models. These Global Earth System Models comprise multiple components, representing a diverse set of physical phenomena and employing different types of discretizations adapted to the particular scales and features of the underlying physical phenomena. As a result, the coupling of these components requires information exchanges (remap) between codes, which involve fields defined on different types of meshes and possibly having different representations, e.g., finite element vs. finite volume, or node-centered vs. cell-centered. Typically, the coupling takes place over a shared subdomain boundary, resulting in interface discretizations that are generally mismatched. For such couplings, a mesh-free approach to data transfer offers an attractive alternative to traditional, mesh-based remap. In this talk we present a flexible data transfer tool, employing Generalized moving least squares (GMLS), and which can handle a wide range of "native'' field representations. GMLS is a meshless reconstruction technique for approximating a target functional from nearby neighbor information, which makes it particularly well-suited for our purposes. The GMLS data transfer tool is based on the recently developed Compadre meshless toolkit, which provides a wide range of utilities for mesh-free discretizations of PDEs. Compadre utilizes the Trilinos software stack to balance workloads over processors, execute k-d tree searches, reconstruct functionals using GMLS, and to provide many additional capabilities for meshfree PDE discretizations. The talk will highlight the ability of the toolkit to also support coupling codes such as components of Earth system models, by allowing for processor assignment of coordinates or sites where information is needed from the peer program. This information is constructed using neighbor information in the peer program and then transferred back. Transfer in this way allows for completely independent distributions of field data in each code being coupled. Numerical results will be presented demonstrating approximation error, global extrema preservation, and global conservation.

Title: Computational Peridynamics with Application to Additively Manufactured Ceramics

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Abstract: Some additively manufactured ceramics are fabricated by depositing a slurry, which consists of alumina powder mixed with a polymer and acid in our work, in lines to form layers. The desired final geometry determines the deposition pattern of lines and layers to build the part. Heterogeneities at the microscale that form during deposition may grow during drying and sintering into flaws that deteriorate materials properties; thus it is important to know which and how flaws limit macroscale materials properties. In this talk, I will show that meshfree peridynamics is a viable approach for modeling key microstructural features of additively manufactured ceramics and their influence on macroscale material response. The focus is on the construction of a meshfree discretization that resolves microstructural features, and application of the Peridigm code to model the effects of thermal and mechanical loading. The high computational expense, due to the large number of degrees of freedom required to resolve fine-scale features, necessitates an efficient parallel software implementation that scales effectively to large numbers of processors. Critical details include the selection and implementation of the constitutive model and bond-failure rule, application of nonlocal volumetric constraints, calculation of thermal strains, treatment of material interfaces, and construction and solution of the global nonlinear system of equations in the case of implicit time integration.

Title: A novel Real-Space Formulation of Density Functional Theory: Designing next generation magnesium alloys

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Abstract: Density Functional Theory (DFT) has the highest accuracy to cost ratio among all electronic structure methods and provides valuable insight in understanding and predicting a wide range of materials properties. Defects in crystalline solids, play crucial role in determining macroscopic properties of materials. The profound significance of defects underlies from the coupling between the discrete effects of the lattice, chemical effects of the core and the long range effects of the elastic field. While DFT is capable of accurately describing the chemistry of the defect core, but are too complicated and expensive for defects with long range fields, methods capable for describing long-range fields rely on empiricism and lack fidelity. This poses an outstanding dual challenge to simulate defects from first principles. To overcome this, we develop a novel coarse-grained formulation of DFT. We employ Linear Scaling Spectral Quadrature method to solve for the electronic fields and develop a coarse-graining strategy based on updated Lagrangian method to describe the long-range fields. We discuss a real space formulation based on high-order finite differences, local reformulation of electrostatics, reformulation of the atomic forces and a parallelization strategy based on domain decomposition method. The developed formulation is sublinear scaling with respect to the system size and has to potential to efficiently simulate defects in crystalline materials from first principles.

Title: A high-order Lagrangian method based on material points and piecewise polynomial maps

Presenter: Nathaniel Morgan
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Abstract: Lagrangian hydrodynamic codes are widely used to simulate gas and solid dynamics. The hydrodynamic methods commonly used in Lagrangian codes are up to second-order accurate, are prone to mesh tangling on large deformation problems, and are not necessarily well suited for advanced architectures that have heterogeneous processors like GPUs. Advanced architectures are forcing algorithmic development to move towards higher compute intensity methods with excellent data locality and internal parallelism. One such method is the high-order discontinuous Galerkin (DG) method. To achieve high-order accuracy, Lagrangian DG methods are combined with high-order elements that have edges/faces that bend. A challenge is that a map to a reference element is required for the deformed high-order elements that are a function of the exterior (and potentially interior) degrees of freedom. The hydrodynamics community would benefit from the development of new high-order Lagrangian methods that do not use the deformed element, and that have favorable properties for advanced computing architectures.

We will present a new high-order total Lagrangian hydrodynamic method that does not need to explicitly track or use the deformed elements as is done in traditional Lagrangian (CG and DG) hydrodynamic methods. The state variables (e.g., density, velocity, and specific total energy) reside at the material points that are updated by solving the governing equations in the initial coordinates using a high-order DG method. We transform the governing equations back to the initial configuration from the deformed configuration using the inverse of the deformation gradient. The deformation gradient is approximated with a piecewise high-order polynomial Pk that is evolved forward in time using a high-order DG method in the initial coordinates. Using the deformation gradient differs from the material point method (MPM), which maps the state at the material points to an underlying mesh where the governing evolution equations are solved. Similar to MPM, the new total Lagrangian method does not use the deformed mesh to solve the governing equations. Likewise, we do not use an isoparametric map based on the deformed element as is done in traditional finite element methods (CG and DG). The superior accuracy of the new Lagrangian method will be demonstrated using a suite of test problems covering both smooth flows and shock driven flows.

Title: A Co-Designed Library for Exascale Particle Simulations

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Abstract: In this talk we will present work to date on the design and implementation of a library for particle simulations within the Exascale Computing Project (ECP) Co-Design Center for Particle Applications (CoPA). Within CoPA, particle-based HPC algorithms spanning a range of applications within ECP are represented including molecular dynamics simulations of materials, particle-in-cell simulations of plasmas and particle accelerators, material point method simulations of additive manufacturing systems, and N-body methods for cosmology. As a co-design center we have identified core computational motifs shared amongst all of these applications and aim to encapsulate portable and performant implementations of these motifs within a library targeting the latest DOE computational platforms. Progress to date on designing and implementing his new library, Cabana, will be presented. This presentation will include an overview of the co-design center, the computational motifs we have identified amongst our application partners, the core data structures of the library, and some algorithm implementations. In addition, we will discuss our use of the Kokkos programming model for portable performance and present some preliminary results meant to emphasize capability on heterogeneous architectures.

Index (presenter and first two co-authors)