**IP1**

**Computational Science Challenges from Petascale and Exascale Computing**

The last year has seen the arrival of Petascale computing and two systems in the top 500 list of supercomputers now exceed a Petaflop in sustained performance. Architecture design for Exascale computing is now already active. Because of fundamental technology constraints, Petascale and Exascale systems will contain very large numbers of independent core counts and much more limited memory bandwidths. This presentation will review the architecture trends for Petascale and Exascale computing and will survey some key algorithms widely uses in computational science to assess the impact and challenges of emerging supercomputer architectures on algorithm performance.

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**IP2**

**Co-evolving Complex Networks: Epidemics in Social and Wireless Networks**

Complex Networks are pervasive in our society. Realistic biological, information, social and technical networks share a number of unique features that distinguish them from physical networks. Examples of such features include: irregularity, time-varying structure, heterogeneity among individual components and selfish/cooperative game-like behavior by individual components. Furthermore, the network structure, the dynamical process on the network and the behavior of constituent agents co-evolve over time. The size and heterogeneity of these networks, their co-evolving nature and the technical difficulties in applying dimension reduction techniques commonly used to analyze physical systems makes reasoning, prediction and controlling of these networks even more challenging. Recent quantitative changes in high performance and wireless computing capability have created new opportunities for collecting, integrating, analyzing and accessing information related to such large complex networks. The advances in network and information science that build on this new capability provide entirely new ways for reasoning and controlling these networks. Together, they enhance our ability to formulate, analyze and realize novel public policies pertaining to these complex networks. The talk will focus on elements of network and information science required to support policy informatics as it pertains to epidemic processes in social and wireless networks. Understanding these epidemiological processes is of immense societal importance. Additionally they serve as excellent "model organisms" for developing a theory of co-evolving complex networks. Perhaps more intriguing, recent advances in wireless communications provide compelling reasons for studying these networks together. I will discuss this possibility in my concluding remarks.

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**IP3**

**Simulation-Based Engineering Science: The Growing Revolution in Modern Engineering and Scientific Discovery**

Science, from the Latin scientia, meaning "knowledge", is the systematic acquisition of knowledge generally about our physical universe. It rests on two fundamental pillars: theory and observation, and the two may be intermingled in complex ways. The pillars describe how knowledge is obtained. Engineering is the application of scientific knowledge to the needs of humankind. Engineering Science the acquisition of knowledge for the purpose of applying it to the needs of humankind. Today, virtually every aspect of our day-today existence is affected by advances in engineering science, – our longevity and quality of life, health, sciences, communication, transportation, and the competitiveness of our nations industry. With the advent of high-performance computing and with major advances in computational science and mathematics, a third pillar of science and engineer science has emerged which may be one of the most significant events in human history computer modeling and simulation. Simulation-Based Engineering Science (SBES) can provide knowledge of events that cannot yet be observed and can explain the ranges of multiple theoretical hypothesis with enormous clarity and precision. Thus it extends traditional boundaries of science and offers possible applications not dreamed of only a few years in our past This lecture reviews the challenges of SBES, describes recent advances, and postulates the remarkable strides in science and technology that could be in store for future generations if these barriers are overcome.

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**IP4**

**Numerical Optimization in Engineering Applications**

Several processes in engineering are subject to optimization, e.g. reducing cost, enhancing effectivity, increasing speed etc. Typically, such optimization problems are quite complex, nonlinear, high dimensional and often involve stochastical influences. Even though the mathematical theory of optimization is quite advanced, not so much is known in such 'realistic situations. We show some industrial optimization problems and indicate the mathematical structure of these problems. We show that relatively simple numerical optimization schemes already give rise to enormous improvements, but we also indicate that the use of such simple methods is limited. In order to overcome such limitations, we describe three techniques, namely automatic differentiation, reduced basis methods and parameter-dependent optimization.

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**IP5**

**Perspectives on Verification, Validation, and Uncertainty Quantification**

Verification and validation (V&V) are the primary means to assess accuracy and reliability in computational simulations. Code verification deals with the assessment of the reliability of the software coding and the numerical algorithms used, while solution verification deals with numerical error estimation of the solution to the mathematical model. Validation assesses the physics modeling accuracy of a computational simulation result by comparing with experimental measurements. Uncertainty quantifica-

tion attempts to characterize uncertainties in the mathematical model and in the experimental data. More difficult questions of uncertainty quantification deal with model updating/calibration and extrapolation of the model to conditions for which no experimental data are available. This talk will briefly discuss all of these issues within the framework of how computational simulations are used in a decision-making environment.

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**IP6**
**Brains, Meaning and Corpus Statistics**

How does the human brain represent meanings of words and pictures in terms of the underlying neural activity? This talk will present our research using machine learning methods together with fMRI brain imaging to study this question. One line of our research has involved training classifiers that identify which word a person is thinking about, based on the image of their fMRI brain activity. A more recent line involves developing a generative computational model that predicts the neural activity associated with arbitrary English words, including words for which we do not yet have brain image data. This computational model is trained using a combination of fMRI data associated with several dozen concrete nouns, together with statistics gathered from a trillion-word text corpus. Once trained, the model predicts fMRI activation for any other concrete noun appearing in the tera-word text corpus, with highly significant accuracies over the 100 nouns for which we currently have fMRI data.

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**IP7**
**Computational Approaches to Multiphysics Applications: Predicting an Object's Thermal Response Within a Turbulent, Reacting, Participating Media Radiation Environment**

Established in 1995, the Advanced Simulation and Computing (ASC) Program supports the Department of Energy's (DOE) National Nuclear Security Administration (NNSA) Defense Programs' shift in emphasis from test-based confidence to simulation-based confidence. Under ASC, computer simulation capabilities are developed to analyze and predict the performance, safety, and reliability of nuclear weapons and to certify their functionality. To serve the ASC Science-Based Stockpile Stewardship Program (SBSS), Sandia National Laboratories (SNL) is actively developing an engineering mechanics simulation capability to predict thermal response of objects exposed to fire enviornments in complex geometries. A fire accident scenario is characterized by the complex coupled physics of turbulent fluid mechanics, combustion, soot generation and transport, participating media radiation (PMR), thermal conduction and in the case of propellant fires, reacting Lagrangian particles. Characterization of abnormal thermal environments, such as those found in fires, is of key importance to ensure safety of weapon systems. This presentation will provide an overview of the math models and numerical coupling approach implemented within the SNL's ASC SIERRA Mechanics code project that supports the engulfed object-in-a-fire scenario.The code is a component of a multi-mechanics framework and is based on a domain-decomposition, message-passing approach to parallel computing. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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**IP8**
**Infectious Disease, Heterogeneous Populations and Public Healthcare: The Role of Simple Models**

Control of infectious diseases in human populations is commonly attempted either by vaccination of uninfected individuals or by effective treatment of those already infected. Both have their limitations: vaccination programmes can be hindered if they cannot reach a sufficient number of individuals whilst treatment programmes are limited by the availability of healthcare professionals to administer such treatment. In addition to these limitations, spread of infectious diseases in humans can be complicated significantly by the social contact structure of the population. In this talk, I will present three caricature models which we have used to explore the potential of simple models to provide useful insights on the effectiveness of public healthcare strategies using HPV and gonorrhoea as case study examples.

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**IP9**
**Experimental Mathematics, Multicore Processors and Highly Parallel Computing**

Multicore processors, incorporated into highly parallel computer systems, are well-suited for the emerging discipline of "experimental mathematics", namely the application of high-performance computing technology in mathematical research. In particular, these systems are well-suited for doing computations to very high precision numerical precision (dozens, hundreds or even thousands of digits), and then, in many cases, analyzing results using techniques such as integer relation detection, to determine if these values are given by simple mathematical formulas. We will present numerous examples of this methodology in action, including applications in supernova simulations, climate modeling, n-body atomic structure calculations, Ising theory, quantum field theory, as well as some notable results in mathematics.

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**CP1**
**Computational Methods Developed for Analysing Porous Particle-Polymer Composites with Complex Microstructures**

Particle based composites comprising nano- and microscale porosity are ubiquitous. The work presented herein concerns the development of computational methods. In particular, algorithms have been developed to mimic mi-

crostructural complexity. This was possible using a voxel matrix approach coupled with morphological dilation/erosion algorithms. These microstructures were then characterised statistically. CFD simulations were used to relate microstructure to permeability and tortuosity, and finite element simulations used to calculate the mechanical properties of these complex composites.

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**CP1**

**A Strategy for Developing General Parallel Boundary-Element Codes**

By expressing a problem solution directly as a function of its boundary values, Boundary Element Methods (BEM) have become an interesting alternative for modeling 3D complex regions as e.g. very large domains or also the microstructure of general composites. In this work, a Krylov-solver-based BE subregion-by-subregion algorithm, which allows modeling a generic number of coupled solids and developing general parallel scalable BE codes, is presented and has its efficiency verified by analyzing three-dimensional carbon-nanotube-reinforced composites.

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**CP1**

**Phase-Field Simulations of Free-Volume Growth in Eutectic Colonies with Coupled Heat and Solute Diffusion**

A quantitative phase-field model is used to investigate the free-volume microstructural pattern formation of eutectic colonies with coupled heat and solute diffusion. The effects of thermal diffusity on morphological instability wavelength in free growth are formulated by simulating the dynamics of fully developed colonies. The model reduces to the traditional sharp-interface model in a thin-interface limit, where the microscopic interface width is small but finite. Finally the model results are compared with isothermal free-volume growth.

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**CP1**

**Stable and Efficient Second-Order Finite-Difference Nonlinear-Multigrid Method for the Phase Field Crystal Equation**

We present a new second-order unconditionally energy-stable finite difference scheme for the Phase Field Crystal equation. In this scheme, the discrete energy is bounded by its initial value for any time step. The equations at the implicit time level are nonlinear but represent the gradients of a strictly convex function and are thus uniquely solvable, regardless of time step-size. We solve the nonlinear equations using an efficient nonlinear multigrid method. The results of numerical experiments are presented and confirm the efficiency and accuracy of the schemes.

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**CP1**

**SquID: A Squared Interatomic Distance Parameterization of Empirical Force Fields in Molecular Modeling**

We discuss a parameterization of empirical force fields in molecular modeling that uses squared interatomic distances rather than atomic coordinates. The additional degrees of freedom introduced decouple the complicated effects of varying the locations of individual atoms, resulting in a more tractable energy minimization problem. In particular, nonbonded interaction terms assume a much simpler form. A nonconvex rank constraint on the metric matrix enforces consistency of the interatomic distances with an actual configuration of atoms.

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**CP1**

**Reduced Basis Method for Nanodevices Simulation**

Ballistic transport simulation in nanodevices, which involves self-consistently solving a coupled Schrödinger-Poisson system of equations, is usually computationally intensive. Here, we propose coupling the reduced basis method with the subband decomposition method to improve the overall efficiency of the simulation. By exploiting *a posteriori* error estimation procedure and greedy sampling algorithm, we are able to design an algorithm where the computational cost is significantly reduced. In addition, the computational cost only grows marginally with

the number of grid points in the confined direction.

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**CP1**

**Morphological Evolution and Coarsening Process of a Strained Heteroepitaxial Thin Film During Constant Deposition**

Self-assembly semiconductor nanostructures such as quantum-dots are a promising inexpensive and effective approach to manufacture novel nanoscale electronic devices. We study the morphological evolution of a strained heteroepitaxial thin film, during continuous mass deposition, on a substrate. Here, we present a new approach for modeling strongly anisotropic crystal and epitaxial growth using regularized, anisotropic Cahn-Hilliard-type equation possessing a source term as a model for the growth and coarsening of thin films. A key feature of our approach is the development of a new formulation in which the interface thickness is independent of crystallographic orientation. We present 2D and 3D numerical results using an adaptive, nonlinear multigrid finite-difference method.

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**CP1**

**Iterative Solution of Generalized Eigenvalue Problems from Optoelectronics with Trilinos**

We study the iterative solution of generalized Hermitian eigenvalue problems arising from the finite-element discretization of $\mathbf{k}\cdot\mathbf{p}$ models of optoelectronic nano systems. We are interested in computing the eigenvalues close to the band-gap which determine electronic and optical properties of a given system. Our work is based on the Trilinos project which provides an object-oriented software framework of integrated algorithms for the solution of large-scale physics problems. Trilinos enables users to combine state-of-the-art eigensolvers with efficient preconditioners, sparse solvers, and partitioning methods. Our study illustrates these possibilities and evaluates various algorithms for their suitability in the context of our physical problem setting.

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**CP2**

**Fast Reconstruction Methods for Diffuse Imaging with Many Sources**

In this work, we address a 2d tomography problem, where we try to reconstruct the absorption coefficient of an elliptic PDE from boundary measurements induced by a large number of sources. We consider a square geometry where the light sources and measurements are located regularly on opposite sides of the domain. The problem in this form requires solving a large nonlinear inverse problem, where the forward problem is given by multiple elliptic PDEs, and is thus computationally intensive. To address this, we propose to solve a linearized version of the problem based on the Born approximation and show that substantial gains can be made in computation. By revealing the special structure of the problem, we design fast methods to assemble the coefficient matrix for the linearized problem. We also propose fast matrix-vector product routines that can be used to solve the linear system with iterative methods or sparse SVD. Finally we introduce a fast inversion algorithm that produces the solution of the inverse problem by solving a sequence of small systems. We demonstrate the effectiveness of our method with several examples.

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**CP2**

**Numerical Methods for Experimental Design**

While experimental design for well-posed inverse linear problems has been well studied, covering a vast range of well-established design criteria and optimization algorithms, its ill-posed counterpart is a rather new topic. The ill-posed nature of the problem entails the incorporation of regularization techniques. The consequent non-stochastic error introduced by regularization, needs to be taken into account when choosing an experimental design. We discuss different ways to define an optimal design that controls both an average total error of regularized estimates and a measure of the total cost of the design. We also introduce a numerical framework that efficiently implements such designs and natively allows for the solution of large-scale problems.

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**CP2**

**Bayesian Multiresolution Method for Local X-Ray Tomography**

A Bayesian multiresolution model for local tomography is proposed. In this model a wavelet basis is used to represent the x-ray attenuation density of the tissues and the prior information is modeled in terms of Besov norms. The

number of unknowns in the local tomography problem is reduced by abandoning fine-scale wavelets outside the region of interest (ROI). This multiresolution approach allows significant reduction in the dimensionality of the image reconstruction problem without loss of reconstruction accuracy inside the ROI. The feasibility of the proposed method is tested with two-dimensional (2D) examples of local tomography in dental radiology.

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**CP2**

**Optimal Member Selection for Large Scale History Matching Using Ensemble Kalman Filter**

Ensemble Kalman Filters have gained increasing popularity for history matching and continuous reservoir model updating. I explore some critical issues related to history matching a large field with substantial production history using EnKF. These include optimal initial member selection while maintaining the required spread in their dynamic response, covariance localization to remove spurious covariance calculations, and application of grid computation for distributing computational requirements. The approach is applied to the Weyburn field, a large carbonate reservoir in Canada, for history matching both water and carbon-dioxide injection phase.

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**CP2**

**Parallel Fully Coupled Two-Level Domain Decomposition Algorithms For Inverse Problems**

This presentation summarizes our work on recovering coefficients of elliptic PDEs. Primarily, optimization and regularization methods are adopted to solve these ill-posed problems. To solve the corresponding nonlinear systems, fully coupled Lagrange-Newton-Krylov algorithms are developed. As the key step in these effective algorithms, several domain-decomposition based two-level preconditioners are employed. Particularly, our algorithms are applied to the problems containing discontinuous coefficients. The advantages of our algorithms and their parallel performance are reported at the end.

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**CP2**

**How Well Can You Hear the Shape of a Drum at a Rock Concert?**

Accelerator cavity shape deviates from design due to lax fabrication tolerances and the tuning process for the accelerating mode. The adjoint method applied to regularized minimization of the least-squares misfit from experimentally measured frequencies estimates the true cavity shape. Using the Laplacian eigenvalue problem posed on a nearly circular 2D region as a simple model, we study the propagation of both measurement error and regularization error to the determined shape using a Bayesian estimation method.

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**CP2**

**Sensitivity Analysis of the Solutions to the Forward Problem of EEG**

The Forward Problem of EEG consists in calculating the electric potential u in the head for a given intracerebral source configuration. We study the sensitivity of u with respect to the conductivity values of the different tissues. Traditional Sensitivity and Generalized Sensitivity are developed and numerical experiments are presented. The information provided by both sensitivities is compared.

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**CP2**

**Gradient Consistency for Discontinuous Galerkin Discretizations of Inverse Problems**

We discuss gradient consistency for discretizations of optimization problems by discontinuous Galerkin finite elements (DG-FEM). To ensure that consistent gradients are obtained from the discretization of the infinite-dimensional optimality system, certain requirements on the DG-FEM discretization must hold. We demonstrate for a model inverse problem governed by nonstationary pure convection that, without gradient consistency, incorrect solutions result.

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**CP3**

**A Finite-Volume Method for Solving Parabolic Equations on Logically Cartesian Curved Surface Meshes**

We present a second-order, finite-volume scheme for the constant-coefficient diffusion equation on curved, parametric surfaces described via smooth or piecewise smooth mappings on logically Cartesian meshes. Our method does not require analytic metric terms, shows second-order accuracy, can be easily coupled to existing finite-volume solvers for logically Cartesian meshes and handles general mixed boundary conditions. We present numerical results demonstrating the accuracy of the scheme, and then use the scheme to solve advection-reaction-diffusion equations modeling biological pattern formation on surfaces.

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**CP3**

**Finite Element Method Used To Study Ellipsoidal Worm Gearing**

Ellipsoidal worm gearing are internal gears derived from globoidal worm gearing, where the worm is placed inside the wheel. The mathematical model of the ellipsoidal threads is the support to obtain surface or solid models, using programming in CAD systems environment. Finite Element Method is used to analyze the behavior of the worm tread surface in contact with the wheel teeth.

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**CP3**

**A High-Order Method for 3D Nonlinear Elastodynamics**

Spatial high-order accuracy and temporal unconditional stability are crucial for accurate and long-time simulations of dynamic nonlinear structural problems involving large deformations. We present a high-order method employing Jacobi polynomial-based shape functions, as an alternative to the typical Legendre polynomial-based shape functions in solid mechanics, for solving 3D dynamic nonlinear elasticity equations. For time integration, we present a composite scheme combining a generalized BDF scheme and the trapezoidal rule for nonlinear elastodynamic equations. The main advantage of the new composite scheme lies in its unconditional stability, simplicity, and the symmetry in the resultant tangential stiffness matrices. We demonstrate the spatial exponential convergence rate and temporal second-order accuracy of the method for the four classes of problems of linear/geometrically-nonlinear elastostatics/elastodynamics. Several 3D nonlinear elastodynamic problems involving large deformations will be employed for comparison with existing algorithms.

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**CP3**

**A Moving Window Algorithm for Parallel Short-Range Wakefield Computations in Particle Accelerators on Unstructured Grids**

Moving window technique on the finite-difference grid is commonly used in simulating short-range wakefields in accelerators to reduce computational requirements. We present the first parallel moving window algorithm on unstructured grid with higher resolution and increased speed. This capability has been developed to allow h or/and p refinement with curvilinear tetrahedral meshes and incorporated into SLACs 3D time domain solver. Application to tapered accelerator cavity shows a tenfold reduction in execution time and memory usage.

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**CP3**

**Interior Penalty Discontinuous Galerkin Methods with Bilinear Immersed Finite Elements (IFE)**

We discusses a bilinear immersed finite element space for interface problems. This space is nonconforming and its partition can be independent of the interfaces. The interpolation error estimates indicate that this space has the optimal approximation capability. Then this space is implemented to two interior penalty DG methods, which use a structured mesh with refinement wherever needed, especially around the interfaces. Numerical examples and convergence analysis show that these methods have the optimal convergence rate.

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**CP3**

**An Optimal Numerical Scheme for PDEs Using Sobolev Norm Minimization**

We introduce a novel interpolation scheme that shows point-wise convergence for a wide class of functions, independent of sample point placement. Furthermore, the scheme has a certain minimax optimality. We use this scheme to develop pseudo-spectral methods for solving ODEs and PDEs, that exhibit a convergence independent

of sample point placement. We also develop fast solvers for these methods. Overall, our methods show spectral convergence and provide fexibility in choice of sample points.

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**CP3**

**Analysis of a Mixed Finite-Volume Discretization of Fourth-Order Equations on General Surfaces**

We study a finite-volume method for the numerical solution of a model fourth-order partial differential equation defined on a smooth surface. The discretization is done via a surface mesh consisting of piecewise planar triangles and its dual surface polygonal tessellation. We provide an error estimate for the approximate solution under the H1-norm on general regular meshes. Numerical experiments are carried out on various sample surfaces to verify the theoretical results.

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**CP3**

**Hierarchical Reconstruction for Discontinuous Galerkin Methods for Solving Hyperbolic Conservation Laws on Unstructured Grids**

The hierarchical reconstruction is applied to the piecewise quadratic discontinuous Galerkin method on 2D unstructured triangular grids. We show that on triangular grids, the use of center biased limiter functions is essential. We develop a WENO-type linear reconstruction in each hierarchical level, which is essentially independent of the local mesh structure. We demonstrate that the procedure can generate essentially non-oscillatory solutions while keeping the resolution and desired order of accuracy for smooth solutions.

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**CP4**

**Parallel Molecular Dynamics Simulation Method Using Multigrid**

Molecular dynamics simulation plays an important role in computational science. We developed a method treating the important long-ranged electrostatic potential, exploiting the fact that the problem can be consistently reformulated as the solution of the Poisson equation. To solve the PDE we use multigrid, resulting in an overall complexity of $\mathcal{O}(\mathcal{N})$. The whole method has been parallelized using MPI and tests on the supercomputers at the Jülich Supercomputing Centre show a very good scaling behavior.

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**CP4**

**Iterative Solvers for Large Sparse Complex Quadratic Equations Arising from Multi-Scale Quantum Simulation of Strongly Correlated Materials**

The parquet formalism to calculate the two-particle Green's function of large clusters requires the solution of a large sparse complex system of quadratic equations. If Newton's method and nf Matsubara frequencies are used, the Jacobian has $O(8{N_f}^3)$ variables and $O(40{N_f}^4)$ complex entries. The Jacobian is not stored but matrix-vector products can be computed directly. We evaluate several Krylov iterative methods for solving large complex Jacobain systems for $N_f \geq 64$. The submitted manuscript has been authored by a contractor of the U.S. Government under Contract No. DEAC0500OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

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**CP4**

**Automatic Runtime Linear Solver Performance Optimization in PDE-Based Simulations**

We propose an automatic adaptive control online system to optimize $PDE$-based simulator performance by dynamically adjusting linear solver parameters during the simulation using solver runtime performance measurements to guide the search. This software system has been successfully integrated into ExxonMobils proprietary reservoir simulator $EM^{powerTM}$. The system can handle large number of combinations of solver parameters, and consistently improves runtime performance of real simulation models, frequently by 30 percent or more, compared to the performance with default solver settings.

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**CP4**

**Combinative Preconditioning Based on Relaxed Nested Factorization and Tangential Filtering Preconditioner**

The problem of solving block tridiagonal linear systems arising from the discretization of PDE on structured grid is considered. Nested Factorization preconditioner introduced by Appleyard et. al. is an effective preconditioner for certain class of problems and a similar method is implemented in Schlumerger's widely used Eclipse oil reservoir simulator. In this work, a relaxed version of Nested Factorization preconditioner is proposed. Effective multiplicative/additive preconditioning is achieved in combination with Tangential filtering preconditioner.

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**CP4**

**Block-Oriented Preconditioners for Fem Modeling of the Drift-Diffusion Equations for Semiconductors**

Various physics-based and approximate block factorization preconditioners are applied to the drift-diffusion equations for modeling semiconductor devices. The resulting scalar subsystems are solved by algebraic multigrid techniques. Blocking by unknowns allows less expensive smoothers. We discretize the drift-diffusion equations with a stabilized finite element method. The nonlinear coupled system is solved with a parallel preconditioned Newton-Krylov method. Preliminary results will be presented demonstrating the performance of these preconditioners compared with one-level and multilevel preconditioners. This work was partially funded by the DOE NNSA's ASC Program and the DOE Office of Science AMR Program, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000

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**CP4**

**Interval Newton Method For Solving Nonlinear Systems Arising in Frictional Contact Problems**

The interval Newton method can be used to solve a system of nonlinear equations and to obtain the preconditioner that is an approximate inverse of the centre of the interval Jacobian. In case when the solution set is bounded or unbounded, directly applying and interval version of the interval Gaussian elimination or the interval Gauss-Seidel algorithm, generally leads to catastrophic overestimation. In this situation, the system must be generally preconditioned.

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**CP4**

**New Truncated ILU Smoothers for Geometric Multigrid Preconditioning of the Convection-diffusion Equation**

We present a numerical study for the effectiveness of using a truncation procedure, similar to the dependence principle used in AMG, for ILU smoothers in the context of multigrid preconditioning of the discrete convection-diffusion equation. Numerical tests in 2D and 3D demonstrate robustness with respect to mesh size, Peclet number and the stretching of the grid. At the same time, the computational resources and the execution times compare very favorably to the standard ILU(0) smoother.

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**CP4**

**Multiscale, Long-Term Analysis of Mico-FSI in**

**Complicated Domains**

Some microfluidics-structure interaction problems are governed by the interplay of the Navier-Stokes equations and Brownian motion. The viscous fluid and stochastic modulation require for a fine spatial and temporal resolution. Yet, we want to analyse the long-term, long-range behaviour. Such multiscale two-physics simulations lead to data masses. Postprocessing becomes a bottleneck. Switching from fire-and-forget semantics to a demand-driven data analysis and simulation steering, we show how it benefits from a FAS solver's multiscale representation.

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**CP5**

**Cluster Computing for Kinetics Models of High Explosive Materials**

Cluster computing for finite-element simulations of three-dimensional, transient, laser-initiated heat transfer in and thermal ignition of confined energetic materials are discussed. The parallel model utilizes PETSc, the Portable, Extensible Toolkit for Scientific Computation from Argonne National Laboratory. Optimal parallel numerical algorithms and cluster computing strategies for modeling the thermo-chemical response of energetic composites under confinement within the current framework are outlined, and model results are presented.

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**CP5**

**Determination of Mechanism and Kinetics of Coal Combustion in Oxygen Enhanced Conditions Using Mathematical Model**

Analysis of kinetics and mechanism of coal combustion processes is presented. This analysis is based on both, the data acquired during an experimental investigation and based on the mathematical model. The combustion process was considered to be carried in gas mixtures, for which the oxygen contents varied between 21% to 100%. The model was developed through the analysis of the rate of mass loss of the fuel sample in the test facility.

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**CP5**

**Numerical Analysis of Crack Induced Debonding Mechanisms in FRP-RC Strengthened Structures**

In this study, the results of a comprehensive numerical investigation are presented to asses the failure mechanisms caused by different types of intermediate flexural and shear crack distributions in reinforced concrete (RC) beams strengthened with fibre reinforced polymer (FRP) composites. The model is based on a bilinear bond-slip relationship with softening behaviour to represent the FRP-concrete interfacial properties. A discrete crack approach is employed to simulate crack propagation through a nonlinear fracture mechanics based finite element analysis to investigate the effects of crack spacing and interfacial parameters such as stiffness, local bond strength, and fracture energy on the initiation and propagation of the debonding and structural performance. Results from the analysis reveal that the debonding behaviour and load-carrying capacity are significantly influenced by interfacial fracture stiffness and crack spacing.

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**CP5**

**Offline and Real-Time Simulation of Vehicle Drivetrain Dynamics**

Computer simulation is an important helpful tool in the virtual prototyping and construction process of cars. One wants to use the same models and data with refinements on the different steps of the process. This leads to specific requirements and numerical treatment to be efficient and accurate for offline as well as the online simulation on testbed systems. Offline developed controllers should work online properly, and online problems should be able to be analyzed offline.

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**CP5**

**Numerical Studies of Heat Transport For Polymer Electrolyte Fuel Cell Stack In Sub-Freezing Environment**

Two cases of heat transfer processes for a general polymer electrolyte fuel cell (PEFC) stack in a sub-freezing environment are studied in this paper: cool-down and heat-up. We investigate the time consumption problem for both of these two cases in order to find the way to normally restart fuel cell stack without regard to electrochemical reaction. We preliminarily consider the action of heat transfer in lieu of generated chemical energy, where the thermal stress/strain and deformation are illustrated as well to show the importance of thermal effect on fuel cell materials. In the numerical simulation, we define a combined finite element - upwind finite volume discretization to approximate the heat transport equation for different cases of heat transport process, and obtain the stable and reasonable numerical solutions. These results correspondingly provide explicit ways to preserve heat in PEFC stack in the sub-freezing environment.

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**CP5**

**Study on Numerical Simulation of Railway Vehicle-Track Dynamic Interaction**

A numerical simulation of interaction between railway vehicles, track and supporting structure plays a very important role in the investigation of track deformations and the dynamic forces acting between train wheels and rails. In this simulation, from the point of view of modeling and computational methods, there exist very interesting problems due to the existence of the high-speed moving contact points and the stiff relationship in the interaction derived from the Hertzian contact theory. Recently a very efficient direct integration method has been developed for the simulation when a contact force is expressed by the linearized Hertzian contact spring model. In this case a numerical simulation is reduced to solving at each time step of the integration, a time-variant, large-scale sparse linear system and carried out efficiently by applying the well-known Sherman-Morrison-Woodbury formula for updating inverse of the coefficient matrix. Also in the simulation of the vibrating test facility excited by the actuator, the stabilization method of J. Baumgarte for so-called differential-algebraic equation has been successfully applied. In this paper, including above results, a recent study on the application of the various computational methods such as an iterative method and a multigrid method, to the simulation of the extended model of the railway vehicle-track dynamic interaction is described.

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**CP5**

**Multiscale Modeling of Thermal and Stress Characteristics of Lithium-Ion Batteries**

Li-ion battery materials have complex particle-to-particle geometries. Several orders of length and time scales span from the microscopic (particle size) to the macroscopic (battery size) scales, resulting in extremely challenging task to conduct first-principle simulations even based on the continuum physical models. In this study, we start with the modeling of single cathode particles to improve our understanding of the physics associated with electron and ion transfer, heat generation and transfer, stress generation and electrochemistry. As a linkage between microscopic and macroscopic scales, a mesoscale simulations on a representative volume element consisting of finite number of particles are conducted to provide volume averaged quantities (such as volumetric reaction rate and effective material properties) to help address the closure problem present in the macroscopic equations.

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**CP6**

**CPOPT: Optimization for Fitting CANDECOMP/PARAFAC Models**

Tensor decompositions (e.g., higher-order analogues of matrix decompositions) are powerful tools for data analysis. In particular, the CANDECOMP/PARAFAC (CP) model has proved useful in many applications such as chemometrics, signal processing, and web analysis. The problem of computing the CP decomposition is typically solved using an alternating least squares (ALS) approach. We discuss the use of optimization-based algorithms for CP, including how to *efficiently* compute the derivatives necessary for the optimization methods. Numerical studies highlight the positive features of our CPOPT algorithms, as compared with ALS and Gauss-Newton approaches.

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**CP6**

**A Probabilistic, Semi-Supervised Classification Algorithm for Large Remotely Sensed Images**

The iterative guided spectral class rejection (IGSCR) classification algorithm is a semi-supervised remote sensing classification method. This work describes a probabilistic version of this algorithm, and details the necessary changes to produce soft classification output. IGSCR uses an iterative clustering method to associate unlabeled data with labeled data, and statistically determines which clusters are used to train a supervised decision rule. Furthermore, the algorithm is specifically designed to be suitable for large, high dimensional datasets.

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**CP6**

**Dynamic Mode Decomposition of Experimental Data**

The decomposition of data taken from numerical simulations into dynamically relevant structures such as global modes has become a standard tool in quantifying time-dependent processes. The same type of analysis is not possible for experimental data due to the lack of an underlying model required by the decomposition algorithms. A new data-based decomposition method is introduced that overcomes this problem and allows the analysis of experimental data; it will be demonstrated on a variety of flow field measurements.

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**CP6**

**The Inductive Algorithms of Model Generation**

One of the important problems in scientific data mining is the problem of regression modeling. To make a regression model using measured data a researcher examines set of competitive models and chooses a model of the best quality. Due to the nature of the experiments non-linear models are common in biological simulations. Symbolic regression allows dealing with large sets of non-linear models. In the lecture inductive algorithms for model creation and selection will be discussed.

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**CP6**

**Using Matrix Methods to Solve Reverse K-Nearest Neighbor Queries**

A reverse k nearest neighbor (RkNN) query q is to find all the objects for which q is in their k nearest neighbors. The current approaches to solve this problem are all based on index tree structures which mostly deal with low dimensional data because of the the dimensional curse. We propose an algorithm by using matrix decompositions such as SVD, CUR, etc. which works good for static high dimensional data set, especially for sparse data. We showed that the amortized cost of our algorithm is superior to the current algorithms based on trees.

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**CP7**

**Simulation of the Behavior of Heat-Shrinkable Thin Films**

We describe a model for the behavior of heat-shrinkable thin films that includes both membrane and bending energies when the thickness of the film is non-zero. We relate the model to those in which a membrane energy or a bending energy are obtained by Γ-convergence techniques. We also provide computational results using the model.

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**CP7**

**Minmaxgd a Software Tools to Handle Series in (max,+) Algebra.**

Industrial processes are characterized by phenomena such as delays, synchronization, concurrency. Such systems can be represented by dynamical models in (max,+) algebra. The input output behavior is then given by ultimately periodic series which represent both transients and periodicals behavior. We will present "MinMaxgd" a software library, interfaced with Scilab, allowing to handle these series. The algorithms complexity will be discussed and method allowing to simulate large systems behavior will be proposed. To deal with uncertain systems, an extension using both interval analysis and (max,+) algebra is also proposed.

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**CP7**

**Agent-Based Computational Modeling of Communication Service Market**

Economic simulation modeling became, in the course of the past decade, a major research direction, allowing the testing of macroeconomic models and theories. Significant attention has been paid to the so-called agent-based economic modeling. In that paradigm, economy is modeled as an evolving system of autonomous interacting agents. Here, the economic agents are considered as driven by rational decisions, possibly subject to noise, that operate aiming to optimize the perceived utility. Within this modeling framework, the dynamics are derived from the first principles, following the assumptions on the utility functions, thus becoming the primary determinant for the actions of the economic agents. We applied this logic to economic activities at the level of an industry, specifically, telecommunication consumer markets. In our model, customers purchase communication services offered by the service providers who compete for the market share, but ultimately for the profitability. The results lead us to the characteristics of interests, such as comparative market positions of different firms. In this paper, we focus on a scenario where the wireless service providers offer mobile targeted advertisement platform. We discuss the potential impact of such a platform on the wireless service market.

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**CP7**

**Adaptive-Fem Simulation and Optimization of the Laser Welding Process**

We present a model for the deep penetration laser welding process. It includes the vapor channel formation, the heat diffusion and the thermo-plastic parts. The results of an Adaptive-FEM implementation for a butt-weld geometry will be shown and compared with experiments. This calibrated simulation of the welds is then used to find the optimum parameters, producing the best weld seams and the least residual stresses. Results of some optimized welds

will also be presented.

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**CP7**

**Numerical Scattering Analysis of Te Plane Waves by a Metallic Diffraction Grating with Local Defect**

We consider the numerical scattering of plane waves by a metallic diffraction grating with a single defect. The diffracted field is solved by applying pseudo-periodic boundary condition on cell boundaries. On the defect cell the perturbed scattered field is obtained by solving the governing wave equation with absorbing boundary conditions derived by a fast recursive doubling procedure. On the rest of the domain it is computed by using the recursive matrix operators efficiently.

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**CP7**

**Effect of Spatiotemporal Elastic Waves on a Driven Thin Plate in Ultrasonic Welding**

Ultrasonic welding uses high frequency mechanical vibrations to produce a solid-state metallurgical bond (weld) between metals. We analyze and simulate the acoustic wave propagation and the energy distribution during ultrasonic welding by a time-dependent elastic model. Our numerical computational results show an energy distribution on the plate that agrees surprisingly well with the experimental results.

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**CP8**

**Deterministic Propagation of Model Parameter Uncertainties in Compressible Navier-Stokes Calculations**

In this lecture, we consider the deterministic propagation of statistical model parameter uncertainties in numerical approximations of nonlinear conservation laws with particular emphasis on the Reynolds-averaged Navier-Stokes equations. As a practical matter, these calculations are often faced with many sources of parameter uncertainty. Some example sources of parameter uncertainty include empirical equations of state, initial and boundary data, turbulence models, chemistry models, catalysis models, radiation models, and many others. To deterministically model the propagation of model parameter uncertainty, stochastic independent dimensions are introduced, see for example Xiu and Karniadakis [D. Xiu and G.Karniadakis, "Modeling uncertainty in flow simulation via generalized polynomial chaos", JCP, Vol. 187, 2002]. Piecewise polynomial basis representations are constructed in these new independent dimensions and the resulting discretized conservation law systems are then solved using a multilevel domain decomposition solution technique. Numerous computational examples in 1-D, 2-D, and 3-D are presented in the full paper to demonstrate accuracy and capabilities of the proposed method.

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**CP8**

**Objective Knowledge Or Subjective Belief?**

The goal of this talk is to clarify what and where the subjectivity in the Bayesian approach lies. Characteristic to Bayesian statistics and its applications to inverse problems is the employment of certain computational techniques such as Markov Chain Monte Carlo methods or variational Bayes methods to explore the posterior densities, to the point that a work not relying on these methods is not even considered Bayesian. In this talk, the point of view is almost completely on the interpretation of the probability, and the use of it to set up likelihoods and priors, while the algorithms in the examples are, characteristically, non-Bayesian. Indeed, exploring the posterior densities and a true statistical inference are hardly not touched upon. This rather eclectic choice is meant to emphasize the possible integration of statistical and traditional numerical methods taking vantage of both of them.

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**CP8**

**Fast Algorithms for Uncertainty Estimation and Propagation in Large Scale Linear Dynamical Systems**

We consider the problem of estimating and propagating the uncertainty in the initial condition field of a convection-diffusion problem describing the transport of atmospheric contaminants. Estimation of the uncertainty is treated within a Bayesian framework. Standard Markov chain Monte Carlo approaches are intractable for such high-dimensional problems. Even when the data and prior uncertainty are Gaussian, and as a result the posterior estimate is Gaussian with covariance given by the inverse of the Hessian matrix of the regularized least squares objective, the computation of the exact covariance matrix is intractable due to the large size and extreme cost of forming the inverse of the Hessian. In the case of linear ill-posed inverse problems, we show that fast algorithms can be constructed that provide accurate low rank Hessian approximations of the least squares data misfit, and as a result permit estimation and propagation of the uncertainty for large-scale problems at a small multiple of the cost of solving the forward problem. Large-scale examples demonstrate the main ideas.

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**CP8**

**Simulation of Stochastic Mesoscopic Models for Self-Organization in Materials**

Self-organization of components of two phase mixtures through diffusion is known as Ostwald ripening. One way of describing this phenomenon is through mesoscopic models; these models are stochastic partial differential equations that have been derived from the microphysics underlying the system. In this talk, results from simulations using spectral schemes for stochastic partial differential equations are described and convergence properties of the method discussed. The simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law.

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**CP8**

**Numerical Solution of Nonlinear Parabolic Partial Differential Equations by Branching Stochastic Processes**

Initial value and initial-boundary value problems for nonlinear one-dimensional parabolic partial differential equations are solved numerically by a probabilistic method. This is based on a probabilistic representation of solutions by means of branching stochastic processes. Most important is a domain decomposition that can be realized. This method allows for a massively parallel implementation, is scalable and fault tolerant. Numerical examples, including some for the KPP equation and beyond are given.

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**CP8**

**Approximating Stochastic Boundary Conditions for Incompressible Fluid Flows**

The two-dimensional cavity and cylindrical vortex breakdown problems have been two widely studied problems in fluid dynamics. Newly developed techniques guarantee higher-order accuracy of solutions. Using a finite difference scheme, we investigate the effects of varying boundary conditions. We introduce noise into the system via the Reynolds' number that is dictated by a circulant finite-state Markov chain. Due to the order-of-magnitude differnces in time-scale between the solution and the random process, direct simulation is impractical. We investigate the validity of the aproximation to an integral Markov process and find that, for white noise, we obtain vastly different results for the two comprable problems.

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**CP8**

**Projection Schemes for Linear Elliptic Partial Differential Equations on Random Domains.**

We present numerical methods for solving linear elliptic partial differential equations on random domains. The fundamental idea is to discretize the governing PDEs using a stochastic mesh representation of the random domain with fixed connectivity but randomly parameterized vertices. The resulting random algebraic equations are solved for the solution statistics using stochastic projection schemes. We present a theoretical analysis of conditions that must be satisfied by the random domain to ensure well-posedness of the problem.

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**CP8**

**Meshfree Solutions to PDEs by Stochastic Programming**

A random search based meshfree method is introduced for determining the solutions to partial differential equations (PDEs). Discretization based approaches to solutions of PDEs have well-known weaknesses which motivates the research of alternative numerical methods. Examples include genetic based algorithms with which the novel algorithm presented here compares favorably in terms of both numerical accuracy and convergence speed. The idea underling the algorithm is based on stochastic programming that finds solutions as linear combinations of candidate solutions. Examples presented include linear, nonlinear and elliptic PDEs.

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**CP9**

**Practical Error Analysis of Numerical Solutions to the Extended Fisher-Kolmogorov (EFK) Equation**

In this talk, I like to discuss, how long time error estimates are obtained using non-traditional methods for the Extended Fisher-Kolmogorov (EFK) Equation

$$u_t + \gamma\Delta^2 u - \Delta u = u - u^3.$$

Traditional methods for analyzing exact error propagation depends on the stability of the numerical method employed. Whereas, in this talk the analysis of the exact error propagation uses evolving attractors and only depends on the stability of the dynamical system. The use of the smoothing indicator yields a *posteriori* estimates on the

numerical error instead of a *priori* estimates.

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**CP9**

**The Fast Multipole Method and Periodic Boundary Conditions in 1D, 2D and 3D**

In this talk we present our error-controlled FMM implementation to treat both homogeneous and clustered particle systems with periodic boundaries. Based on a renormalization approach all multipole interactions from the periodic image cells with the cubic simulation cell are precomputed independently of the actual particle distribution. Additionally, we show results and timings of high-precision computations as well as large-scale computations with more than 2 billion particles and a comparison to available Ewald summation schemes.

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**CP9**

**A Poisson-Like Model of Sub-Clinical Signs from the Neurological Examination of Healthy Aging Subjects**

Based on the presence or absence of clusters of sub-clinical neurological symptoms, six independent signs are derived. Using a health aging population, logistic regression is employed to generate density functions for each sign which are then used to construct a Poisson-like model of the distribution of number of signs observed for this population as a function of age. This allows the simulation of a longitudinal population with the same characteristics as the original population. One main result is for this population, the number of signs observed increases linearly with age after age 62. This model also allows for the comparison of the neurological aging process in different groups over a long time period groups that may vary by disease status, prescription drug use, or diet.

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**CP9**

**On a Numerical and Mathematical Analysis of the Random Differential Quadrature (RDQ) Method**

A novel strong-form meshless method called the random differential quadrature (RDQ) method is presented, which extends the applicability of the differential quadrature (DQ) method over an irregular domain containing uniform or randomly distributed field nodes. Convergence and consistency analyses of the RDQ method are presented using 1-D, 2-D and elasticity problems as test cases. Von Neumann stability analysis of the DQ method is presented using 1-D wave equation for several single and multi-step schemes.

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**CP9**

**Resolving Multiscale Spatial Features Dynamically**

We introduce a hybrid moving mesh - level set algorithm to dynamically move, and create/delete mesh nodes in one, two and three dimensions. This hybrid algorithm differs from previous h-r hybrid methods in that global properties of the numerical solution are considered for the creation or removal of nodes, allowing for a smoother co-ordinate mapping. This hybrid moving mesh framework is used to simulate fine scale features arising from a one stream plasma instability.

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**CP9**

**A Rational Interpolation Scheme with Super-Polynomial Rate of Convergence**

The purpose of this study is to construct a high order approximation method for arbitrary data points. The resulting function approximation is an interpolation function when the data set is exact, or a regression if measurement errors are present. We represent each data point with a Taylor series, and the approximation error as a combination of the derivatives of the the target function. A weighted sum of the square of the coefficient of each derivative term in the approximation error is minimized to obtain the interpolation or regression approximation. The resulting approximation function is a high order rational function with no poles. When measurement errors are absent, the interpolation approximation converges to the target function faster than any polynomial rate of convergence. Preliminary results show that this scheme naturally extends to multivariate approximations as well.

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**CP9**

**A Far-Field Taylor Series Treecode for Multiquadric Radial Basis Functions**

We present a treecode to evaluate the multiquadric radial basis function (RBF), $\phi(x) = \sqrt{x^2 + c^2}$. In the treecode, the RBF nodes are divided into a hierarchy of clusters and the far field effect of a cluster is approximated using a far-field Taylor series. The Taylor series converges uniformly for $c \geq 0$, which is wider than the Laurent series proposed by previous investigators, which converges on an interval $0 \leq c \leq c_1$, where $c_1$ is proportional to the node spacing. We implement the Taylor series in Cartesian coordinates and compute its coefficients using a recurrence relation. The treecode error, CPU time, and memory usage are reported and compared with direct summation for randomly distributed particles in a cube and on a sphere. For a given order of Taylor approximation, the treecode CPU time scales as $O(NlogN)$ and the memory usge scales as $O(N)$.

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**CP10**

**Automatic Generation of Performance and Power Models for Parallel Scientific Applications**

While the number of tools and experts in performance analysis is growing, the generation of performance models for parallel applications remains a difficult, time-consuming, and largely manual process. We discuss the requirements for automating this process and present a component-based approach for collecting and analyzing performance and power data for parallel scientific applications, including automation of collection, storage, and analysis of performance data and application metadata. This infrastructure enables application developers to analyze and improve the performance of their applications without requiring expert help.

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**CP10**

**Optimizing HPC Applications with Source-Level Reuse Distances**

The advent of chip multiprocessors has brought the problem of memory locality back to the fore with a vengeance in high performance applications. We describe an approach based on a novel source-level metric, called source-level reuse distances, that can be employed by software tools to guide program optimizations more suited to modern processor architectures than those conventionally followed. The methodology is illustrated with examples taken from real programs written in MATLAB.

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**CP10**

**Algorithms for Millisecond-Scale Simulation on a Special-Purpose Molecular Dynamics Machine**

Anton, a recently completed special-purpose machine for molecular dynamics simulations, achieves a speedup of several orders of magnitude over general-purpose systems by mapping novel algorithms to massively parallel application-specific hardware. We describe the algorithms and numerical techniques used by Anton, including some developed especially for Anton and others adapted to exploit its hardware. These algorithms underlie Anton's ability to avoid communication bottlenecks even at high levels of parallelism, to effectively map computation onto fast, specialized pipelines, and to efficiently and deterministically produce accurate results.

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**CP10**

**Conceptual Model Builder (CMB): A New Framework for Model Creation and Initialization**

The US Army ERDC researches, develops, supports, and maintains many discipline-specific numerical models. For many large scale modeling applications, it is no longer feasible to execute the mesh generation, boundary condition assignment, and visualization processes on a single-processor desktop computer. Therefore, a cross-platform framework of tools is being developed to handle pre- and post-processing of large numerical simulations. This talk will discuss the numerous requirements and design decisions for the CMB framework.

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**CP10**

**Design and Implementation of Parallel Simd Algorithm for Finding Complex Roots on the Cell Processor**

We describe the design and implementation of a parallel multicore SIMD algorithm for finding complex zeros of analytic functions in a given region. The main contribution of our work is a new multicore SIMD algorithm for complex root calculations, which has been designed for efficient execution on the SPUs of the CELL Processor. We combine parallel multicore methods for domain decomposition with SIMD evaluations of complex functions, to achieve a high degree of parallelism. Towards this end we have developed a SIMD optimized complex math library. We have effectively used multicore (using 6 SPEs), SIMD (4 complex function evaluations simultaneously), superscalar (dual instruction execution optimization on the SPU), and distributed computing (using a cluster of PS3s), thus combining all facets of parallel programming in our implementation.We compare the performance of our implementation on CELL/SPU with an Opteron 242 SMP multi-threaded implementation. Our SPU based parallel implementation is atleast 25 times faster than the Opteron based solver. We achieve 140 gigaflops on function evaluations and domain decomposition with an SPU efficiency above 90%.

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**CP10**

**Database and Analysis Support for Automated Configuration of Scientific Applications**

Component-based software via the Common Component Architecture (CCA)has proven helpful in managing the complexity of high-performance scientific applications. Recent work focuses on automating application configuration and dynamic tuning to improve performance, that is, ideas on computational quality of service (CQoS). We introduce new database and analysis components that support management and analysis of performance and associated meta information using machine learning techniques. We present results for applications in quantum chemistry and nonlinear solvers.

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**CP10**

**The Use of Connectors in Parallel Simulators with Deep Hierarchical Structure**

Interaction between components can be embodied in the notion of software connectors. Connectors manifest themselves in a software system as a number of functionalities. Especially for parallel systems, connectors become key determinants of system properties, such as performance, scalability, reliability, and so forth. In this work a hierarchical simulator framework (MphyScaS) and its mapping into distributed components among many processes are presented. Connectors were designed to provide desired functionalities for the interaction among those components.

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**CP10**

**Automated Algorithm Generation and Thread Parallelism in Multiphysics Simulation Software**

Traditional programming approaches are algorithm-centric. In multiphysics applications, where models are hierarchical and various models require different transport equations, constitutive laws, and equations of state, algorithms become extremely complex. In this talk I propose a new software design methodology for multiphysics simulation where mathematical expressions are represented directly in the software. Using graph theory, we automatically generate (non-unique) algorithms. This approach has two substantial benefits: 1) it removes complexity from algorithm design, 2) it provides a basis to exploit task-based parallelism (via threads) in a more broadly distributed parallel (MPI) environment.

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**CP10**

**Towards Dense Linear Algebra for Hybrid GPU Accelerated Manycore Systems**

We highlight the trends leading to the idea of hybrid manycore/GPU systems, and a set of techniques that can be used to efficiently program them. The presentation is in the context of Dense Linear Algebra. We also stress on the need for new algorithms that would split the computation in a way that would fully exploit the power that each of the hybrid components offers. We give an LU factorization example of unprecedented performance.

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**CP11**

**Analyzing Stock Market Interval Data with Fourier Transformation**

The overall stock market can be measured with the S & P 500 index. Using interval data and computing rather than traditional point methods, researchers have recently obtained astonishing computational results in studying the variability of the stock market. We further apply discrete Fourier transformation to study the S&P 500 interval data and reveal some interesting behaviors of the market. In this talk, we report our initial findings.

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**CP11**

**Option Price in the Presence of Random Arbitrage Return**

We consider option pricing problems when we relax the condition of no arbitrage in the Black Scholes model. The derived pricing equation is in the form of Stochastic Partial Differential Equation (SPDE). We used Karhunen-Loève expansion to approximate the stochastic term, and the numerical solution of the SPDE is computed using Finite Element Method.

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**CP11**

**Numerical Investigations of Various Forms of the Heston Model**

This research explores comparability of the Heston and Black-Scholes option pricing models by investigating the effects of variations in the Heston model on stability and performance. Analysis focuses on the volatility component, especially modifications to decrease the computations required to price an option by this model. Spectral analysis methods are also used to determine a periodic function that describes volatility comparable to a CIR random process.

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**CP11**

**Computational Complexity of Portfolio Margining**

Calculating regulatory margin requirements for investment portfolios is a critical risk management operation for any prime brokerage firm. Despite the fact that the margin calculation problem was posed more than three decades ago, it remains one of the most notorious problems in financial service industry, and its computational complexity has not been well studied. In this work, we discuss mathematical models of the margin calculation problem and present related theoretical and practical computational complexity results.

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**CP12**

**An Interpolation-Based Approach to the Weighted-$H_2$ Model Reduction Problem**

We present a new formula for the $H_2$ error norm in weighted $H_2$ model reduction problem. This formula illustrates the significance of interpolation at the mirror images of the poles of the weighting system as well as at the mirror images of the reduced and original system poles. We then propose an iteratively corrected interpolation-based algorithm for the weighted-$H_2$ model reduction problem. Several numerical examples are presented to illustrate the effectiveness of the proposed approach.

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**CP12**

**Coupled Matrix Factorizations Using Optimization**

Matrix factorizations are important tools in many data analysis applications: dimensionality reduction, noise reduction, and data fitting, among others. In this talk, we discuss the use of optimization methods for solving the problem of factorizing two or more matrices coupled in some way. Such problems arise, for example, in analyzing bibliometric data containing authors and journal papers, where we want to simultaneously analyze the relationships between papers using both author-document and term-document features.

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**CP12**
**Optimization of Groundwater Flow Models Using Proper Orthogonal Decomposition (pod)**

We are solving inverse problems in groundwater modeling. Given values of hydraulic head at discrete locations, we seek to approximate values of hydraulic conductivity for the entire field. When using ADH, extreme run-times prohibit the frequent function calls needed for parameter estimation for large, complex problems. Proper Orthogonal Decomposition POD is a method to reduce the size of the problem to calibrate ADH, reducing the number of full function calls needed.

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**CP12**
**Inexact Solves in Interpolatory Model Reduction**

We expand upon the work of Beattie and Gugercin, who examined the role of inexact solves in interpolation-based model reduction. We will illustrate the importance of Petrov-Galerkin framework in this setting and discuss the resulting backward error formulation from a systems theory perspective. We show the effect of inexact solves in one-sided and two-sided interpolation-based reduction as well as for the optimal H2 approach. Finally, we investigate effective preconditioning techniques in the model reduction setting.

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**CP13**
**Semi-Lagrangian Time-Splitting Scheme for Atmospheric Models**

A combination of semi-implicit (SI) and semi-Lagrangian (SL) approaches was shown to be efficient numerical technique in atmospheric modeling, because it allows us to circumvent the Courant-Friedrichs-Lewy condition with respect to both fast acoustic-gravity waves and slower advective processes. In this research we apply additional splitting in the context of SISL scheme to reduce the order of linear systems needed to be solved at each time step and speed up their solution.

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**CP13**
**High Order Mimetic Differential Operatos**

Mimetic Operators satisfy a discrete analog of the divergence theorem and they are used to create/design conservative/reliable numerical representations to continuous models. We will present a methodology to construct mimetic versions of the divergence and gradient operators which exhibit high order of accuracy at the grid interior as well as at the boundaries. As a case of study, we will show the construction of fourth order operators in a one-dimensional staggered grid. Mimetic conditions on discrete operators are stated using matrix analysis and the overall high order of accuracy determines the bandwidth parameter. This contributes to a marked clarity with respect to earlier approaches of construction. As test cases, we will solve 2-D elliptic equations with full tensor coefficients arising from oil reservoir models. Additionally, applications to elastic wave propagation under free surface and shear rupture boundary conditions will be given.

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**CP13**
**Dual-Mixed Finite Element Approximation of Stokes and Generalized Stokes Problems**

In this talk a finite element method for a dual-mixed approximation of Stokes and nonlinear generalized Stokes problems is discussed. The method approximates the velocity, its gradient, and the total stress tensor, but avoids the explicit computation of the pressure, which can be recovered through a simple post-processing technique. Existence, uniqueness, and error results for the method are given, and algorithms for solving the linear systems that arise in computations are discussed.

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**CP13**
**Multi-Material Remap for Staggered Discretization**

Remapping is one of the essential parts of most Arbitrary Lagrangian-Eulerian (ALE) methods. In this talk, we present a new remapping method for all fluid quantities in the staggered multi-material ALE framework. It is based on evaluating of high-order material mass fluxes (using intersections), including the corner fluxes, and attaching all quantities to these fluxes. We will focus on remap of nodal quantities, performed also in a flux form. We will show several numerical examples to demonstrate

properties of our remapping method.

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**CP13**

**High Resolution Adaptive Algorithms For Subsurface Flow**

Simulations of subsurface flow play an important role in assessing the long term fate of groundwater contaminants around waste disposal sites, evaluating strategies for carbon sequestration and a variety of other applications. Here, we describe a parallel adaptive mesh refinement framework for high-fidelity simulation of multiphase-multicomponent flow in porous media. Our approach is based on a sequential formulation that treats pressure implicitly, combined with a semi-implicit treatment of convection, diffusion and reactions. We demonstrate the overall methodology and discuss parallel performance on some representative geochemical problems.

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**CP13**

**A High-Order Projection Scheme for Amr Computations of Chemically Reacting Flows**

A high-order projection scheme was developed for the study of chemically reacting flows in the low-Mach number limit. The projection scheme for the momentum transport is coupled with an operator-split stiff approach for the species and energy equations. The code employs a block-structured high-order adaptive mesh refinement approach to tackle the challenges posed by the large spectrum of spatial scales encountered in reacting flow computations. Results for several canonical configurations are used to illustrate the performance of the numerical construction.

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**CP13**

**An Extension of the Discrete Variational Derivative Method to Mixed Meshes by the Mimetic Finite Difference Schemes**

Generally, for PDEs that enjoy conservation or dissipation properties, numerical schemes that inherit these properties are advantageous in that the schemes give qualitatively better solutions in practice. Lately Furihata and Matsuo have developed *the discrete variational derivative method* that automatically constructs conservative or dissipative finite difference schemes on regular rectangular meshes for a class of PDEs with certain variational structures. Employing the mimetic finite difference schemes, we extend this method to mixed meshes.

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**CP14**

**Effects of Terrain Induced Wind Rotors on Pollution Particles**

We will discuss our research on the terrain induced wind rotors found in Owens Valley, California and the effect these rotors have on the transportation and location of pollution particles within the valley. We will do this by discussing our mathematical model of the wind fields of Owens Valley and by visually representing the chaotic behavior of the pollution particles' trajectories as they move through the terrain induced wind rotors.

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**CP14**

**Probabilistic Modeling of Langrangian Particle Trajectories**

Analyzes instantaneous and steady state distributions of particles in a velocity field of atmospheric motion over Owens Valley, California. The instantaneous distribution of particles is a single release of particles. The steady state of particles is a continual release of particles. Determines the location of particles at a given time, the probability of that location, and visualizes the probabilities. Given the velocity field, traces the particle trajectories through the use of the Runge-Kutta code.

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**CP14**

**Three-Dimensional Visualization of Terrain-Induced Rotors**

Our talk will encompass the visual aspects of terrain-induced rotors discovered over Owens Valley, California. We will talk briefly about the valley's unique topography. We also expect to discuss two-dimensional and three-dimensional projections of various atmospheric dynamics directly affected by these rotors. Additionally, we plan to demonstrate the effects these atmospheric rotors have on particle movement and trajectory.

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**CP14**

**The Simulation of Contaminant Transport in Groundwater and Environmental Risk Assessment**

The problem of assessing groundwater pollution has become a matter of considerable concern. For proper groundwater management, it is necessary to model the contamination mathematically in order to assess the effects of contamination and predict the transport of contaminants. Several deterministic models have been proposed and numerical procedures developed. Because of aquifer heterogenity, the the spatial variation of flow properties is erratic. Therefore a stochastic model of flow regime and transport processes is more realistic. In this talk we use a new method (*A. Beskos and G.O. Roberts*, Exact simulation of diffusions, The Annals of Applied Probability 2005, vol. 15(4), 2422-2444) for modelling contaminant transport. Furthermore we adress sensivity analysis of exceedance probabilities with respect to variations of the transmissivity field, porosity and dispersivity.

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**CP14**

**A Coupled Wave, Current, and Seabed Morphology Approach for Coastal Process Simulation**

In order to accurately simulate multi-physics coastal ocean processes, the wave action equation, the shallow-water equations, and the Exner equation are coupled in a simultaneous manner. A flux-limited version of the Roe scheme is derived to discretize the coupled system for high-resolution solutions. Numerical experiments will be presented for validations of the scheme, and example simulations such as evolution of a wind driven sand dune will be demonstrated for the performance of the coupling system.

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**CP14**

**Visualization of the Xz Tauri Protostar Jet**

The starting point for this project is the two-dimensional simulations by Gardner and Dwyer of the temperature, density, and radiative cooling of the proto-astrophysical jet XZ Tauri. We explore methods of visualizing the data as well as three-dimensional data generated from the original data. Techniques include visualization of isosurfaces for the three-dimensional representations and use of colormaps for the two-dimensional representations. We also made three movies of the evolution of the jet.

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**CP15**

**An Infinite-Dimensional QR Algorithm**

We show how the classical QR algorithm can conceptually be adapted to solve spectral problems for infinite matrices representing bounded operators on separable Hilbert spaces. When the infinite matrix $A$ has $k$ subdiagonals, we propose a numerical algorithm that computes, in finitely many flops, the leading $m$-by-$m$ submatrix of the infinite matrix that results from $n$ applications of the QR algorithm on $A$. Applications abound since most operators in physics act on infinite-dimensional spaces.

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**CP15**

**Automatically Constructing Sparse Preconditioners for High-Order Finite Element Systems**

High-order FEs have many advantages over linear FEs for a large class of problems. Unfortunately the corresponding matrices and subsequent multilevel preconditioners are costly to store, which has shown to be limiting in many cases. However, memory can be reduced by using sparse representations of these dense matrices during the preconditioning stage. We present recent convergence results for a method that automatically constructs sparse preconditioners using the high-order FE stiffness matrices.

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**CP15**

**New Krylov-Space Solvers for Symmetric Positive Definite Matrices with Indefinite Preconditioners**

Incomplete LDLT factorizations sometimes produce an indefinite preconditioner even when the input matrix is symmetric positive definite. The two most popular iterative solvers for symmetric systems, MINRES and CG, cannot use such preconditioners; they require an SPD preconditioner. We present two new Krylov-subspace solvers, a variant of MINRES and a CG-like algorithm, which can be preconditioned using any non-singular symmetric matrix as long as the original system is SPD. These algorithms allow the use of incomplete-factorization preconditioners for SPD systems, even when the preconditioner is indefinite,

and without resorting to a more expensive non-symmetric iterative Krylov-space solver.

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**CP15**

**Unassembled HyperMatrix Project Status Report**

We present a strategy for sparse direct factorization for the matrices arising from hp-adaptive FEM. The proposed algorithm is based on the element hierarchy, which is generated by local refinements of elements. Our method stores the matrices as un-assembled element matrices in a tree structure according to the refinement history. Benefits of the new data structure and algorithm include a ordering of unknowns motivated by the refinement history, an ability to update part of an existing factorization when a local refinement occurs, and a natural identification of supernodes. We describe how the new approach more naturally supports FEM and present performance data.

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**CP15**

**Optimization and Parallelization of FIND Algorithm**

The FIND algorithm is a fast algorithm to calculate entries of the inverse of a sparse matrix. This type of calculation is critical in many applications including quantum transport in nano-devices. We will discuss the algorithm and various optimizations to reduce its computational cost and present two different algorithms to parallelize the calculation. They are based on ideas from cyclic reduction and dynamic programming. The extension to 2D and 3D meshes is particularly challenging. The performance of these algorithms will be compared and discussed.

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**CP15**

**A New Hybrid Method for Finding An Eigenpairs of a Symmetric Quadratic Eigenvalue Problem in An Interval**

The symmetric quadratic eigenvalue problem

$$(\lambda^2 M + \lambda C + K)u = 0,$$

where M, C, and K are given $n \times n$ matrices and $(\lambda, u)$ is an eigenpair, arises in a wide variety of practical applications, including vibration, acoustic, and noise control analysis. In the most practical application, the problem is often of a very large dimension. Unfortunately because of the nonlinearity, the problem is extremely hard to solve numerically. The state-of-art computational techniques, such as the Jacobi-Davidson method, are capable of computing only a few extremal eigenvalues and eigenvectors if the initial vector is chosen properly. Fortunately, there are engineering applications that require only some of the eigenvalues lying within an interval. In this paper, a new Hybrid method combining a Modified Parametrized Newton-type method with the Jacobi-Davidson method is proposed to compute an eigenpair of a quadratic pencil within an interval. The experimental results show that this method is much faster than the Jacobi-Davidson method. The results of this paper generalize those of an earlier work on Parameterized Newton's Algorithm for finding an eigenpair of a symmetric matrix.

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**CP16**

**Scalable Parallel Fluid-Structure Interaction Simulations for Blood Flow**

Computer simulation of blood flow in human arteries is a challenging problem requiring expertise in physiology, medical imaging, and computational modeling. We develop a parallel computational method for the equations of blood flow coupled to a model for the compliant artery walls, and apply this method to simulations of blood vessel geometries derived from patient-specific clinical data. These simulations feature monolithic coupling of fluid and structure in one large system and scalable algorithms suitable for use

on large supercomputers.

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**CP16**

**Computational Model of the Role of Tissue Architecture in Radiotherapy**

Tissues with a healthy architecture, made of stem/progenitor/differentiated cells, behave in ways that are significantly different from those made of tumourigenic cells. This is likely to result in different levels of adaptation to the tumour environment and, as a consequence, to the response to radiotherapy. In this talk I will introduce an agent-based computational model that simulates these two scenarios and discuss its potential application to study cancer and help oncologists design new and efficient therapies.

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**CP16**

**Analysis of a Mathematical Model of Early Brain Tumor Growth**

In this presentation, I give an introduction to the mechanisms involved in early growth of Glioblastomas Multiforme. I then introduce a mathematical model describing tumor growth, blood vessel formation, and growth factors that affect them both. This model is used to predict the behavior of a developing brain tumor and investigate the way it forms. The model demonstrates different growth behaviors based on varying initial conditions, model parameters, and growth assumptions.

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**CP16**

**Mathematically Modeling the Mass-Effect of Invasive Brain Tumors**

When developing an accurate model of the development of glioblastomas multiforme, it is important to account not only for the invasion and diffusion of tumor cells into healthy tissue, but also the resulting mass effect and brain tissue deformation. This motivates the model presented here, which implements the finite element method to solve a boundary value problem defined through classical continuum mechanics. Intended to improve existing models of tumor invasion, this model predicts the mass-effect of an invading tumor in heterogeneous brain tissue. Several parameters, taken from existing literature, dictate the behavior of differing types of brain matter. The model operates on a two-dimensional (2D) domain, and outputs the displacement of brain tissue as a result of peri-tumor pressure.

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**CP16**

**Interaction of Tumor with Its Microenvironment: A Mathematical Model**

In order to understand the role of fibroblasts and myofibroblasts in the early induction of breast cancer in vitro, we developed a mathematical model to simulate interactions between these fibroblasts and tumor epithelial cells as well as performed experiments to validate the model. The mathematical model describes the dynamics of various concentrations of cells and growth factors present in the tumor microenvironment by a system of partial differential equations. In the experiments, tumor cells are placed on one side of a membrane and either normal fibroblasts or tumor associated fibroblasts are placed on the other side. This membrane is semi-permeable, allowing growth factors such as EGF and TGF-beta to cross over, however restricting cells from being in direct contact with each other. Simulation of our mathematical model and results from our experiments were in good agreement and therefore confirmed the models ability to predict aspects of tumor cell behavior in response to signaling from fibroblasts.

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**CP16**

**Mathematical Modelling and Numerical Simulation of Non-Newtonian Flow with Application in Hemodynamics**

Blood is a complex, non-Newtonian fluid-solid mixture which consists of deformable cells, e.g. red blood cells (RBCs) that are suspended in an essentially Newtonian plasma. Blood's microstructure, in particular the RBCs, imply the non-Newtonian behaviour. The blood exhibits the shear-thinning property, i.e. breakup of RBCs at low shear, viscoelasticity -due to the cell deformation and cell aggregation and shear anisotropy-due to the alignment of cells with the flow direction. In the present work we use the macroscopic model that reflects the shear-thinning blood property. In particular we work with the power-law type model of the Carreu and the model with Yeleswarapu viscosity. Our aim is to study the blood flow in elastic vessels. In practice the deformation of elastic artery wall is not negligible and can lead to localized reversal flow which implies a formation of arteriosclerotic plaques and stenosis - inner lumen constriction of the vessels. The mathematical model is based on the fluid-structure interaction between the shear-thinning fluid and elastic vessel. The deformation of the blood vessels is modelled by the gen-

eralized string equation which yields a second order differential equation for the wall displacement. The interaction between fluid and structure is twofold. First, the structure enforces a non-homogeneous Dirichlet-type boundary condition on the wall. Moreover, the fluid enforces the movement of the vessels and thus we have in the string equation the forcing term induced by the fluid stress tensor. The coupled problem is solved iteratively by means of the strong coupling between the fluid and structure. Study of hemodynamical wall parameters confirms the importance of using the non-Newtonian rheology in order to get reliable predictions of arterosclerotic plugs.

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**CP16**

**Afem for Parametric Surface Flows: Applications to Biomenbranes.**

When lipid molecules are immersed in aqueous environment they aggregate spontaneously into 2 mono-molecular layers or (bio)membranes that form an encapsulating bag called vesicle. This happens because lipids consist of a hydrophilic head group and a hydrophobic tail, which isolate itself in the interior of the membrane. As a first approach, we have studied a model based on geometry assuming that the equilibrium shapes are the minimizers of the Willmore energy under area and volume constraints. In this context, the membrane is the preponderant factor influencing the shape of the vesicle. A gradient flow is established to reach these equilibrium shapes. Then, the effect of the inside (bulk) fluid is taken into account leading to more physical dynamics. The boundary conditions couple Stokes equations to the constrained Willmore force. A parametric approach is employed, which leads to forth order highly nonlinear PDEs on surfaces and involves large domain deformations. An adaptive finite element method, with either piecewise linear or quadratic polynomials, is used for both the geometric and coupled problems.

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**CP16**

**A Multiscale Model of Thrombus Development**

A 2D multiscale model is introduced for studying formation of thrombus in a blood vessel. It involves components for modeling viscous, incompressible blood plasma; platelets; blood cells; activating chemicals; fibrinogen; the vessel walls and their interactions. The macroscale dynamics of the blood flow is described by the continuum NS equations. The microscale interactions between platelets, platelets and fibrin(ogen) and platelets and the vessel wall are described through a stochastic discrete Cellular Potts Model. We also make predictions about different stages in thrombus development which can be tested experimentally and suggest specific experiments.

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**CP17**

**Nested Iteration First-Order System Least Squares on Incompressible Resistive Magnetohydrodynamics**

Magnetohydrodynamics (MHD) is a fluid theory that describes Plasma Physics by treating the plasma as a fluid of charged particles. Hence, the equations that describe the plasma form a nonlinear system that couples Navier-Stokes with Maxwell's equations. To solve this system, a nested-iteration-Newton-FOSLS-AMG approach is taken. Most of the work is done on the coarse grid, including most of the linearizations. We show that at most one Newton step and a few V-cycles are all that is needed on the finest grid. Here, we describe how the FOSLS method can be applied to incompressible resistive MHD and how it can be used to solve these MHD problems efficiently in a full multigrid approach. A 3D steady state and a reduced 2D time-dependent test problem are studied. The latter equations can simulate a "large aspect-ratio" tokamak. The goal is to resolve as much physics from the test problems with the least amount of computational work. We show that this is achieved in a few dozen work units (A work unit equals a fine grid residual evaluation).

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**CP17**

**Numerical Modelling Of Mhd Flow Of A Micropolar Fluid Past A Stretched Permeable Surface With Heat**

Input your absThis work considers steady, laminar, MHD flow of a micropolar fluid past a stretched semi-infinite, vertical and permeable surface in the presence of temperature-dependent heat generation or absorption, magnetic field and thermal radiation effects. A set of similarity parameters is employed to convert the governing partial differential equations into ordinary differential equations. The obtained self-similar equations are solved numerically by an efficient implicit, iterative, finite-difference method. The obtained results are checked against previously published work for special cases of the problem in order to access the accuarcy of the numerical method and found to be in excellent agreement. A parametric study illustrating the influence of the various physical parameters on the skin friction coefficient, microrotaion coefficient or wall couple stress as well as the wall heat transfer coefficient or Nusselt number is conducted. The obtained results are presented graphically and in tabular form and the physical aspects of the problem are discussed.

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**CP17**

**Simulation of Fast Magnetic Reconnection in**

**Anisotropic Two-Fluid Collisionless Plasma**

We present multiscale simulations of fast magnetic reconnection using an anisotropic collisionless two-fluid plasma model for the (microscale) magnetic diffusion region and magnetohydrodynamics for the macroscale model. We implement each model using a shock-capturing third-order discontinuous Galerkin solver. This includes a study of the terms in the generalized Ohm's law.

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**CP17**

**A Projection Method for Discretized Electromagnetic Fields on Unstructured Mesh**

Projected discretized electromagnetic fields on another mesh can serve as an initial guess to get the more accurate answer. A new method for projecting discretized electromagnetic fields on one unstructured mesh to another is proposed. Two examples are used for studying the errors of different projection methods. The analysis shows that the new method is very effective on balancing both the error of the electric field and that of the magnetic field.

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**CP17**

**Implementation and Verification for Fully Conservative Lagrange-Remap Modeling of MHD Shock Propagation**

Two classical verification problems from shock hydrodynamics are adapted for verification in the context of ideal magnetohydrodynamics (MHD) by introducing strong transverse magnetic fields, and simulated using the finite element Lagrange-remap MHD code ALEGRA for purposes of rigorous code verification. The concern in these verification tests is that inconsistencies related to energy advection are inherent in Lagrange-remap formulations for MHD, such that conservation of the kinetic and magnetic components of the energy may not be maintained, and inconsistencies in shock propagation may therefore arise. That kinetic energy is not conserved in standard Lagrange-remap formulations is well known, and the correction of DeBar has been shown to eliminate the resulting errors. Here, the consequences of the failure to conserve magnetic energy are revealed using order verification in the two magnetized shock-hydrodynamics problems. Further, a magnetic extension to the DeBar correction is proposed and its accuracy evaluated using this verification testbed. Results indicate that only when the total energy is conserved, by implementing both the kinetic and magnetic components of the DeBar correction, can simulations in Lagrange-remap formulation capture MHD shock propagation accurately, such that shock wave speeds and jump conditions are correctly computed, and errors converge at the expected rate. Implications for the implementation of the DeBar correction are drawn from the results as well, including the use of certain limiters on the correction and the required accuracy of the remap scheme.

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**CP18**

**Partitioned Time Stepping Algorithms for a Parabolic Problem on Two Subdomains**

Various physical models feature equations on two domains coupled through an interface condition, requiring parallelizable algorithms to estimate the solutions. We consider two heat equations posed in domains $\Omega_1, \Omega_2 \subset \mathbf{R}^2$ adjoined by an interface $I = \Omega_1 \cap \Omega_2 \subset \mathbf{R}$, and coupled by a condition that conserves energy dissipation across $I$. Stability and convergence results are derived for a partitioned time stepping approach and an implicit-explicit (IMEX) approach, (where the data on $I$ is lagged), verified by numerical experiments.

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**CP18**

**Parallel Computing for Long-Time Simulations of Calcium Waves in a Heart Cell**

The release of calcium ions in a heart cell can lead to diffusion waves and is modeled mathematically by a system of transient reaction-diffusion equations. To enable long-time simulations, efficient and physically accurate high-order time-stepping methods are vital. I will show how a special-purpose code captures the crucial physical effect of self-organized wave initiation. Performance studies on a distributed-memory cluster also demonstrate the excellent scalability of the code.

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**CP18**

**On the Stability of a Numerical Scheme for a System of Differential Equations with a Large Skew-Symmetric Component**

Numerical methods for the solution of a system of differen-

tial equations dominated by a skew-symmetric component suffer from a time step size that approaches zero in order to satisfy stability conditions. We introduce a new explicit method that has demonstrated, numerically and analytically, increased stability without forcing the step size to zero. The new method is modeled on a predictor-corrector scheme with multiplicative operator splitting.

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**CP18**

**Higher Order Implicit-Explicit Integral Deferred Correction with Additive Runge-Kutta**

We produce higher order implicit-explicit integrators by using additive Runge-Kutta (ARK) methods in the prediction and correction loops of Integral Deferred Correction (IDC). We implement these methods and analyze whether order and stability properties of the embedded ARK method are preserved by IDC. These integrators can be applied to systems of ODEs that contain both stiff and nonstiff terms, resulting from method of lines discretization of certain PDEs, e.g. advection-diffusion equations.

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**CP18**

**Higher Order W-Methods**

In solving stiff systems of ODES, the efficient methods are implicit in nature. Rosenbrock methods are a class of linear implicit methods for solving such stiff systems of ODEs. In the Rosenbrock methods the exact Jacobian must be evaluated at every step, which can make the computations costly. In contrast, W-methods use occasional calculation of the Jacobian matrix. This makes the W-methods popular among the class of linear implicit methods for numerical solution of stiff ODEs. However the price we have to pay is large amount of work needed to find the coefficients of the W-methods. As the order of the W-methods increases, the number of order conditions of the W-methods increases very fast. This makes the design of higher order W-methods difficult. In this talk, we show how to construct fourth order W-methods.

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**CP18**

**Construction and Performance of Exponential Integrators for Large Stiff Systems of Differential Equations**

Exponential integrators offer computational advantages compared to standard methods in solving large stiff systems. These techniques possess better stability properties than explicit schemes and offer computational savings compared to implicit integrators by requiring fewer Krylov projection iterations per time step. We will discuss what constitutes an efficient exponential integrator and how it can be constructed and analyzed. We will compare performance of several exponential and standard schemes and demonstrate their application in plasma physics and other fields.

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**CP19**

**Tree-Structured Sphere Decomposition**

We are motivated by an optimization problem arising in optical lithography that reduces to a search over a sphere of dimension greater than 2. We summarize a technique for decomposing a sphere of arbitrary dimension into a specific number of regions of equal area and small diameter. We show how a tree-based implementation can provide efficient decomposed forward and reverse lookup into a set of indexed partitions in space.

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**CP19**

**PDE Constrained Optimization for the Design and Quality Control of Accelerator Cavities**

PDE constrained optimization is a key technology for the design, and quality control of accelerator cavities for which the constraint is the large scale Maxwell eigenvalue problem, and the unknown variable is the cavity shape. We present the algorithms that minimize the regularized least squares misfit to achieve the multiple design goals of fixed accelerating frequency, desired field flatness, and small external Qs for the HOMs. Actual applications including the CEBAF 12 GeV Upgrade, Choke Mode cavity and the Crab cavity for LARP will be presented.

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**CP19**

**A Fast Optimization Scheme for the Estimation of Velocity Fields for Geophysical Fluids**

We consider the assimilation of satellite images, within the framework of data assimilation in geophysical systems. Based on the constant brightness assumption, we define a nonlinear functional measuring the difference between two consecutive images, the first one being transported to the second one by the unknown velocity. By considering a multiscale approach and a Gauss-Newton minimization algorithm, we can estimate high-resolution velocity fields at a high frame rate and then assimilate these billions of pseudo-observations.

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**CP19**

**New Robust Control Design Algorithm for Sampled-Data Systems**

A new integrated robust control design method for sampled-data systems is proposed. The method is composed of a new robust finite RHC (receding horizon control) algorithm based on minimax optimization and a new DA (digital-to-analog) conversion method which is consist of interpolation using predicted information calculated in RHC algorithm and switching of the sampling function according to the system status. Numerical example will be given to show the effectiveness of the proposed method.

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**CP19**

**Computation of Lq-Optimal Actuator Locations**

In many problems governed by partial differential equations, the actuator locations can be chosen. In the case of linear quadratic control, and a random initial condition, the trace of the Riccati operator should be minimized. To minimize the response to the worst choice of initial condition, the cost function is the norm of the Riccati operator. Approximations are used in selection of the best actuator locations. The optimal cost and location of the approximating sequence should converge to the exact optimal cost and location. Conditions for this convergence are given, along with examples.

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**CP19**

**Transforming the Linear Regression Residual for Lipschitz Continuity in Genetic Global Optimization Applications**

In quantitative genetics, linear regression of multidimensional problems is frequently used to scan for genetic positions influencing a trait. We show how the stochastic process of inheritance renders an expectation for the Lipschitz constant in the residual function. We then use this result to derive a deterministic termination condition for a Lipschitz-based global optimization scheme. We also show how the result can be used to greatly speed up permutation testing for significance, and consider the applicability to other problems with a stochastic structure.

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**CP19**

**Fast Methods for Mountain Passes**

In computational chemistry and differential equations, we often seek a critical point of a function by finding a "mountain pass" between two given points: a connecting path along which the maximum value is minimized. We describe an algorithm that maintains lower bounds on the optimal value by keeping the two points in separate level set components. We prove convergence, even in the nonsmooth case, and local superlinear convergence in the smooth finite-dimensional case.

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**CP19**

**Integral Equation-Constrained Optimization in 3-D Optimal Shape Stokes Flow Problems**

An integral equation-constrained optimization approach to three-dimensional (3-D) optimal shape problems for a viscous incompressible fluid under the assumption of zero Reynolds number has been developed. It couples the theory of generalized analytic functions with the adjoint equation-based method. The approach has been illustrated for the drag minimization problem for the axially symmetric translation of a solid particle of revolution in the viscous incompressible fluid in an unbounded domain and in a pipe.

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**CP20**

**Large-Eddy Simulation of Turbulent Combustion**

With the recent improvements in the processing speed of computers Large-Eddy Simulation (LES) has emerged as a promising tool for the numerical study of fluid dynamics. The applications of LES range from the aerospace engineering field to the bioengineering field. LES is the Computational Fluid Dynamics (CFD) technique providing time-accurate unsteady solution of complex high Reynolds number flows. Results proofing the successful applicability of LES to the field of aerospace engineering, biosciences and

atmospheric sciences are presented.

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**CP20**

**Global Hydrodynamic Stability Analysis of Large-Scale Compressible Flows Using Krylov Techniques**

A preconditioned Krylov technique is employed to perform a global stability analysis of two hydrodynamic flow problems: a compressible mixing layer and a supersonic flow about a swept parabolic body. This iterative technique is implemented via a Jacobian-free framework where direct numerical simulations provide the required input. It further features a spectral transformation to add flexibility to our global stability solver and to allow access selected parts of the full global spectrum.

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**CP20**

**Simulations of Hot Spot Initiation in High-Energetic Material**

Under mechanical/thermal insults, micron-sized pores embedded in high-energetic materials collapse generating high-temperature regions leading to ignition. Two-dimensional high-resolution mesoscales simulations are performed on an axisymmetric configuration using ALE3D. ALE3Dis a massively parallel multiphysics ALE hydrodynamics software with a large suite of advanced material models. The parameter space is systematically studied by considering various shock strengths, pore diameters and material properties. Key mechanisms for hot spot initiation will be discussed.

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**CP20**

**Dynamics of Vesicles in a Confined 2D Stokes Flow**

The formulation and numerical solution of the dynamics of suspended vesicles in a bounded Stokes flow will be presented. We use a boundary integral formulation for the fluid that results in a set of nonlinear integro -differential equations for the vesicle dynamics. On one hand, explicit time-stepping schemes suffer from a severe stability constraint due to the stiffness related to high-order spatial derivatives. On the other hand, implicit time-stepping schemes can be expensive because they require the solution of a set of nonlinear equations at each time step. To circumvent these difficulties, we employ a semi-implicit scheme that does not have severe stability constraints and whose computational cost per time step is comparable to that of an explicit scheme. We discretize the equations by using a spectral method in space. We report numerical experiments that demonstrate the convergence properties of our scheme.

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**CP20**

**Concerning Use of the Reverse Heat Equation to Solve Field Interpolation Problems for Vortex Methods**

Vortex methods are numerical schemes for approximating solutions to the Navier-Stokes equations using a linear combination of moving basis functions to approximate the vorticity field of a fluid. We explore accurate means of interpolating a known field on a linear combination of overlapping basis functions. This is a necessary problem to address when one is configuring a calculation given a desired initial condition or when one wishes to replace an undesirable configuration of basis functions with a desirable one. We present a new field interpolation method using the reverse heat equation to solve the field interpolation problem. When using high accuracy stencils and integrators, the new method is fast, explicit and high precision. The algorithm is implemented into the open source BlobFlow project which has been parallelized using MPI and verified using MPI-Spin.

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**CP20**

**Artificial Viscosity Proper Orthogonal Decomposition Models**

Many scientific and engineering applications, such as weather prediction and flow control, require both accurate and efficient numerical simulations of turbulent flows. Within these applications, the Smagorinsky eddy viscosity model has played a dominant role in large eddy simulations (LES) over the years. This model, which has been developed around the idea of energy cascade, has proven to be a valuable technique. On the other hand, reduced-order models, such as proper orthogonal decomposition (POD),

emerge as computationally efficient methodologies in the calculation of turbulent flows. In this talk, we present artificial viscosity Galerkin POD models that synthesize ideas stemming from LES and POD. We also present a rigorous numerical analysis supported by extensive numerical experiments.

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**CP20**
**A Stokes Flow Based Roughness Metric**

Our main goal is to predict the effects of boundary roughness on the drag in Navier Stokes flow directly from its topography through analysis of the first and second order shape derivatives of the roughness-to-drag mapping. For the Stokes flow, not surprisingly, analytical derivation shows that a flat wall is a stationary point (a minimum) of this mapping. The eigenfunctions of the shape Hessian of the drag are Fourier modes, and the sensitivity of the drag is approximately linear in the wavenumber. These results provide a metric to evaluate roughness effects, which are also useful for Navier Stokes flow.

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**CP20**
**Prediction of Unsteady Flow Fields Using Higher Order Singular Value Decomposition (HOSVD) and Bi-Orthogonal Proper Orthogonal Decomposition (BPOD)**

The temporal evolution of unsteady flowfields for varying values of the ratio of the density of a tumbling plate to that of the ambient fluid is predicted using the methods of HOSVD and BPOD on snapshots of flowfields obtained from computational fluid dynamics (CFD) simulations. Pressure distributions of tumbling plates obtained from these methods are then validated against CFD simulations and errors assessed. A detailed description of the methods and a comparison of results will be presented during the talk.

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**MS0**
**Title not available at time of publication**

Abstract not available at time of publication.

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**MS1**
**Computing Semi-Classical Quantum Dynamics with Hagedorn Wavepackets**

We focus on techniques for dealing with the curse of dimensionality for the time-dependent Schrödinger equation. We look first at sparse grid techniques and then at the approximation of multi-particle quantum dynamics in the semi-classical regime by Hagedorn wave-packets. Discovered in the context of theoretical semi-classical models in quantum mechanics, these generalisations of the Hermite-functions are particularly suitable for the approximation of the highly oscillatory solutions of the quantum molecular dynamics in many dimensions. We present a time-reversible, fully explicit time-stepping algorithm to approximate the solution of the Hagedorn wave-packet dynamics. The algorithm is robust in the semi-classical limit and allows for the treatment of multi-particle problems by thinning out the basis according to a hyperbolic cross approximation, and of high-dimensional problems by Hartree-type approximations in a moving coordinate frame. The highly efficient implementation is then essential for the arising large-scale computations.

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**MS1**
**Numerical and High Performance Computing Challenges in Quantum Dynamics**

We first give a brief overview of the computational challenges arising in quantum dynamics. Then, we focus on performing large-scale computations where the high-dimensional, time-dependent Schrödinger equation is solved using modern parallel computers with multicore nodes. We present performance results for an optimized OpenMP-MPI implementation using a high-order finite difference scheme on a multi-block grid, and we also show results where the dissociation of a $CO_2$ molecule is simulated using the multi-block solver in an adaptive setting.

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**MS1**

**Time-Propagation for the Schrdinger Equation: A View from Quantum Chemistry**

Several different numerical propagation methods for the time-dependent Schrödinger equation with an explicit time-dependent Hamiltonian are discussed and compared. The propagation schemes are applied to one- and three-dimensional molecular systems where ultra-fast laser pulses couples several molecular states. Of the compared methods, the 4th order Magnus-Lanczos propagator appears to be the best choice.

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**MS1**

**Transparent Boundary Conditions Based on the Pole Condition**

To simulate wave propagation problems posed on infinite domains it is common to introduce transparent boundary conditions. This way the computational domain is restricted to a finite domain, which can be discretized by finite elements or finite differences. The novel pole condition approach, which is based on a Laplace transform of the solution in a generalized radial direction, results in high order approximate transparent boundary conditions that are local in time.

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**MS2**

**Efficient Methods for Solving Robust, Non-stiff Discretizations of the Immersed Boundary Method**

The Immersed Boundary (IB) Method is a versatile tool for the investigation of flow-structure interaction. In a large number of applications, the immersed boundaries or structures are very stiff and strong tangential forces on these interfaces induce severe time-step restrictions for explicit discretization. This excessive stability constraint can be removed with suitable implicit discretizations but at a seemingly prohibitive computational cost. More economical alternatives are limited in their applicability to simple boundaries and interfacial forces. Consequently, the extraordinary structure-building capability of the IB methodology cannot be exploited with these low-cost approaches. Recently a robust, semi-implicit discretization originally introduced by Peskin that is free of numerical stiffness has received renewed attention. In this discretization the spreading and interpolation operators are lagged (i.e. evaluated at the current interfacial configuration rather than at the future one) and leads to a linear system of equations for the interface configuration at the future time when the interfacial force is linear. For nonlinear forces the same linear system or one of similar structure becomes an essential part of Newton-type iterations. In this work we propose efficient iterative methods for solving Peskin's lagged-operators type of discretization. We do this by first constructing a sufficiently accurate approximation to the system's matrix that can be expeditiously obtained by using a combination of pre-computed values and interpolation. The availability of a matrix allows for more efficient matrix-vector products and facilitates the design of a larger class of iterative schemes. We propose efficient iterative methods that can deal with both linear and nonlinear interfacial forces and simple or complex immersed structures with tethered or untethered points. We demonstrate that our approach is several orders of magnitude more efficient than the standard explicit method and we show both the robustness and efficacy of our proposed methodology with a challenging application of a 2D model of a heart valve.

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**MS2**

**Novel Paradigm for Solving PDEs on Non-Graded Cartesian Grids**

In this talk, we will describe recent advances in the field of free boundary problems, with an emphasis on level-set and ghost-fluid methods. We will discuss their applications to two-phase flows with phase-change and to the Stefan problem. Novel methods for adaptive mesh refinement will be discussed as well.

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**MS2**

**Effects of Oscillatory Boundary Motion on an Incompressible Viscous Flow**

Understanding of the effects of oscillatory boundary motion on the behaviour of incompressible fluid flow is very important for the accurate modelling of real-world flow problems. We consider problem of Poiseuille flow in two spatial dimensions, assuming fixed lower boundary while the top boundary experience oscillations. The numerical scheme is based on spatial finite element discretization along with operator-splitting technique for time discretization. The results of numerical simulations suggest dependence of flow rate on nature and frequency of boundary oscillations.

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**MS2**

**A Stable and Efficient Method for Treating Surface Tension in Incompressible Two-phase Flow**

A new approach based on volume preserving motion by mean curvature for treating surface tension in two-phase flows is introduced which will speed up significantly the computations of flows that exhibit stiff surface tension effects. The new method will be easy to implement in the context of level set methods, or coupled level set and volume of fluid methods. The new method will work regardless of the complexity of the interface separating gas from liquid. The new method works in the context of adaptive mesh refinement. Theoretical and numerical justification shall be presented which validate the new approach.

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**MS3**

**Dynamic Load Balancing of 3D Finite Element Particle-in-Cell Code Pic3P**

The successful design and operation of next-generation light sources and accelerators depends strongly on injector performance. SLAC's parallel 3D Finite Element Particle-In-Cell code Pic3P has enabled unprecedented modeling accuracy of space-charge dominated beam-cavity interactions by using conformal unstructured meshes and higher-order particle-field coupling. Adaptive refinement, causal moving window techniques and dynamic load balancing allow solving large problems. This talks presents the methods used that allow Pic3P to scale to thousands of CPUs.

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**MS3**

**Deriving Matrices for Transforming Finite Elements**

While the basis functions for the most widely used kinds of affine finite elements are mapped in a one-to-one fashion from a reference element to each element in a mesh by a simple transformation, more complicated finite element spaces (such as Hermite and Argyris) also require more complicated transformations. For these elements, the images of the transformed basis functions must be "corrected" by a linear transformation applied on each element. The sparsity (or lack thereof) of this transformation is an important factor in how expensive the finite element bases are to use. We will use some classic finite element notions to reason about the structure of the graph of this matrix.

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**MS3**

**Developments in Dense Linear Algebra for Multicore and Hybrid Systems PLASMA Framework**

Development of high performance software for multicore hardware faces multiple challenges. New directions have to be explored to address both performance and productivity issues. The PLASMA dense linear algebra library delivers performance on multicore processors through the use of novel algorithms and data structures and efficient scheduling of parallel tasks. This talk gives a brief introduction to the main concepts behind the PLASMA framework and an then focuses on mechanisms for expressing task parallelism in code and methods for efficient task scheduling.

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**MS3**

**Interconnection Networks for Scientific Workloads**

The increase in number of processors in state of the art supercomputers brings interconnection networks back to the fore. Despite the rich literature in topological properties of interconnection networks, studies on the relation between these topologies and real scientific workloads are sparse and recent. In this talk, we will review recent developments in this area and introduce our architecture simulation framework that will help us study the performances of novel interconnects on real scientific computing applications.

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**MS4**

**Supersonic Turbulence and Star Formation in Molecular Clouds**

Turbulence within molecular clouds generates shock waves that tear the cloud material into a hierarchy of smaller and smaller clumps. It also provides the necessary kick to overcome the outward pressure and cause the densest cloud cores to collapse leading to the birth of stars. This "turbulent fragmentation" is believed to shape the initial mass function of newly born stars. However, scaling properties of highly compressible, magnetized isotropic turbulence that constitute the basis for this new statistical theory of star formation are still poorly understood. In my talk I shall review results from large-scale numerical simulations that investigate the properties of supersonic hydrodynamic and MHD turbulence. Our nonmagnetic simulations are large enough to isolate the inertial range in density and velocity statistics. We find strong departure from the incompressible Kolmogorov velocity scaling at high turbulent Mach numbers. We propose an extension of Kolmogorov's phenomenology to compressible regimes and discuss how magnetic fields modify these results. I will also discuss the effects of large-scale driving force used in the simulations on the derived turbulent statistics, intermittency and fractal dimension of dissipative structures in supersonic turbu-

lence.

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**MS4**

**Numerical Relativity and the Art of Modeling Black Holes and Neutron Stars in Exa-scale Platforms**

One of the most difficult challenges of computational astrophysics is modeling strongly gravitating objects such as black holes and neutron stars. These objects can only be accurately described in the theoretical framework of Einstein's Theory of General Relativity which provides a set of highly non-linear second-order partial differential equations that govern the behavior of the gravitational fields. This poses a problem of much larger complexity than when using Newtonian theory and, until very recently, the basic problem of two black hole systems could not be tackled without employing some sort of approximation. I will cover the recent advances that allowed a phenomenal breakthrough in the field of numerical relativity in the past years and review the challenges that the field faces to take the simulations to exa-scale platforms.

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**MS4**

**3D Simulations of Turbulent Reactive Flows in Stellar Interiors**

Abstract not available at time of publication.

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**MS4**

**Petascale Challenges for Cosmological Simulation**

Abstract not available at time of publication.

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**MS5**

**Fast Algorithms for Applying Multidimensional Green's Functions**

We construct approximations of free-space Green's functions as well as those with Dirichlet, Neumann or mixed boundary conditions on simple domains. For any selected accuracy, these approximations yield fast algorithms for applying multiparticle Green's function, those for Poisson and Helmholtz equations, the Leray projector and other operators of mathematical physics. These algorithms involve convolution with a sum of decaying Gaussians and, in some cases, an additional multiplication by a band-limited kernel in the Fourier domain.

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**MS5**

**An Overview of Some Recent and New Fast Algorithms for Solving PDEs Based on Green's Function Approach**

In this talk, we will first very briefly review the ideas behind some fast algorithms for constant coefficient Elliptic PDEs, mostly based on Green's function approach. Then we will present some classes of problems where these algorithms are suitable as it is. Then we will show how to adapt these algorithms for some non-constant coefficient PDEs and present some numerical results.

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**MS5**

**Non-equilibrium Temperature Modeling in Eulerian Hydrodynamics**

Mixing simulations often use pressure-temperature-velocity equilibrium among material components. For shock driven mixing this assumption is of limited validity, since the time scales for temperature equilibrium are often much longer than those for advective mixing. We discuss a computational study of large amplitude cylindrical implosions, comparing results from pressure-temperature equilibrium with front tracking. We focus on late time behavior of the unstable interface and aspects of the implosion that are influenced by the interface treatment.

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**MS5**

**Efficient Algorithms for Coupling Thermal Radiation Transport to Hydrodynamics**

Radiation hydrodynamics is the study of phenomena where the presence of thermal radiation affects the dynamics of a hydrodynamic system. Representing the joining of two separate fields of computational physics, radiation hydrodynamics presents unique multiscale problems that neither radiation transport nor computational hydrodynamics has in isolation. In this talk I will present recent research into numerical methods for the coupled simulation of radiation hydrodynamics. Specifically, I will explore algorithms to couple the numerical schemes for the different physical operators. This coupling is nontrivial because, in general, discretizations for hydrodynamics and radiation transport are not readily compatible in terms of number of unknowns, and each operator can have spatial and temporal scales differing by several orders of magnitude.

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**MS6**
**Outreach and Education Through Computation**

Computational Science and Engineering (CSE) has emerged as a multidisciplinary field that has empowered scientific and engineering discoveries through computer simulations. Moreover, the development of computer simulation codes have led to breakthroughs that need to be fed back to the CSE community through effective outreach and education. The DOE Advanced Computational Software (ACTS) Collection Project has pursued and implemented mechanisms to bring a set of advanced and portable software tools to be speed up in the development CSE applications. We use software abstractions to transfer the knowledge on state-of-the-art CSE technologies to the community at large.

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**MS6**
**Transforming Petascale Education through HPC University**

HPC University is a virtual organization launched in 2007 focused on high-quality, high-performance computing (HPC) learning and workforce development activities and resources designed to prepare the next generation of science and engineers utilizing petascale computing systems to advance scientific discovery. Participation in this virtual organization is open to all interested organizations that want to help expand the breadth and depth of the range of resources and services as well as to help broaden community involvement. During the SIAM Conference, the HPCU virtual organization will provide an update of the HPCU requirements analysis, implementation, development, and dissemination plans. The team will describe the on-going process of identifying community needs. There will be a question and answer period to solicit additional community input and foster increased collaboration and participation among the community. We invite all interested organizations to join in developing effective strategies for expanding and scaling-up the opportunities to best serve the computational science and HPC needs of research and education communities.

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**MS6**
**Fostering the Next Generation of HPC Researchers Through DOE Computational Science Graduate Fellowship Program**

The DOE Computational Science Graduate Fellowship (CSGF) program provides a unique opportunity for the nation's top Ph.D. students to receive financial assistance, unique training opportunities, and to become a part of a community of computational scientists and engineers. The program began in 1991 and has supported over 250 students who are now working in national laboratories, academia, and industry. The DOE CSGF program supports students in an array of computational disciplines including: biology, physics, materials science, applied mathematics, computer science, aerospace engineering, fluid dynamics, and medical applications. This talk will discuss the requirements and benefits of the program as well as the activities we are conducting to promote the development of the next generation of leaders in high performance computing research.

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**MS6**
**Computational Science and Engineering @ CITRIS and Cal**

Through high performance computing, mathematical modeling and science/engineering thinking, CSE promises a radical and paradigm change in interdisciplinary research and education to understand the nature of the real world complex natural and social systems, to enhance human knowledge from a wealth of large-scale heterogeneous digital-biological data, and to build cyber science model for scientific and social systems to enhance scientific discovery and innovation by bringing people and resources together across geographical and cultural boundaries. In this presentation, I will present the current structure of CITRIS CSE and Cal CSE and to explore common resources within campuses to better educate students and carry out multi-campus research. CITRIS CSE vision is to support the work of the most creative minds in science and engineering as they pursue complex and computationally intensive basic and applied research that will enhance national and international leadership, maintain a competitive edge and improve the quality of life for humanity.

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**MS7**
**Generic Modeling for Detailed Intraorgan Kinetics and Whole Body Distribution**

Pharmacokinetic pharmacodynamic (PKPD) modeling requires a multiscale approach in which one would like to reduce models as expeditiously as possible in order to gain computational speed in analyzing multiple data sets. Toward this end, a generic organ-level model (GENTEX) for tracer and mother substance exchanges and reaction sequences has been incorporated in multiple representations into a Whole Body Model for distribution kinetics (PK) and reactions within individual tissues or organs. On top of this generic structure, we allow individualized programming for the body's responses (PD), including such responses as changes in regional flows that impact the PK part of the systems. Although each GENTEX model can be extended to 13 species, and multiple paths requiring up to 100,000 ODE equivalents (for PDEs), each organ model can be reduced automatically at run time to avoid com-

putations for regions or reactions not used, and can be reduced to a single stirred tank model. Thus models for drugs with complex hepatic clearance can be detailed while leaving the rest of the body simplified.

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**MS7**

**Modeling Blood Flow in the Circle of Willis**

The circle of Willis is one of the few arterial structures in which vessels form a circle, which enable perfusion of both hemispheres despite occlusion of one of the major vessels. In this work we show, using a non-linear one-dimensional viscoelastic fluid dynamic model of the arteries in the circle of Willis, that both hemispheres can be perfused even if one of the major inflow vessels (the carotid) artery is occluded. This model predicts blood flow in the circle of Willis using a network of 16 interconnected vessel segments whose base structure is given from patient specific data. The vessel radii and lengths are obtained from a MRI angiogram from a healthy young subject. Using the ensemble Kalman filtering method we validated the model against transcranial Doppler ultrasound measurements of blood flow velocity for a healthy young subject. Measurements of finger systolic and diastolic values of blood pressure were used to ensure that computed blood pressures were within the right range. Blood flow velocity was measured in the middle, anterior, and the posterior cerebral arteries. Inflow to the model was obtained from blood flow velocity measurements from the carotid and basilar arteries.

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**MS7**

**Pulmonary Pulse Wave Propagation**

We present a numerical model of periodic pulse propagation in the full pulmonary circulation. The arteries and veins are treated as two fully-coupled, bifurcating trees of compliant and tapering vessels. Given cardiac output data and pressure in the left atrium, we study the effects on the pressure pulse waveform of the number of generations of vessels, and of vascular compliance, and assess the possibilities for early detection of disease.

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**MS8**

**Time-Evolving Fluid Interfaces in Multi-Physics Environments**

We present numerical methods for computing the motion of two dimensional bubbles in a slow viscous flow. These bubbles may be immersed in an electric field, or they may be in the presence of soluble/insoluble surfactant. The model is a coupling of the Stokes equations with the Laplace equation. New methods are presented for both the solution of the governing equations and for the time integration of the evolving interfaces. When surfactant is present, the evolution can be stiff and a small-scale decomposition is performed to extract the dominant term in the dynamics. Efficient implicit-explicit methods are then used for the evolution equations. Integral equations are formulated for both Stokes flow and Laplace's equation. These equations are solved using a Fast Multipole-accelerated iterative solver that is spectrally accurate and has optimal efficiency. Several large-scale examples which demonstrate different phenomena are presented.

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**MS8**

**Energetic Variational Approaches in Complex Fluids: Least Action Principles and Maximum Dissipation Principles**

We will exam/employ various variational approaches for those hydrodynamical systems modeling the complex fluids. In particular, we will illustrate the compatibility of

LAP and MDP in these systems.

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**MS8**

**The Dynamics of Multicomponent Inextensible Vesicles in a Viscous Fluid**

We develop a thermodynamically consistent model to simulate the dynamics of multicomponent vesicles. The model accounts for viscous flow, surface phase separation, variable bending stiffness and spontaneous curvature in addition to the line tension between coexisting surface phases phases. We perform simulations of the model using new and efficient boundary integral methods for 2D and 3D axisymmetric vesicles. Simulations are performed that reveal the complex morphologies that result from the many competing effects. For example, we demonstrate that a multicomponent vesicle may tumble in a shear flow under conditions for which a single-component vesicle will reach a steady shape.

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**MS8**

**Numerical Schemes for Complex Fluids**

Models of complex fluids typically couple the momentum equation to an equation governing the evolution of the microstructure. Examples include liquid crystals, fluids containing elastic particles, and polymer fluids. These systems have an underlying Hamiltonian structure which (1) reveals the form of the terms coupling the two equations, and (2) is used to establish stability of the system. This talk will focus on the development and analysis of numerical schemes which inherit the Hamiltonian structure, and hence stability, of the continuous problem. Compactness properties of the discrete solutions will then be presented to establish convergence of these schemes.

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**MS9**

**Multiscale Flux Basis Implementation for a Mortar Mixed Finite Element Method and its use in Stochastic Collocation of Flow in Porous Media**

First we describe an alternate implementation of the mortar mixed finite element method, which is computationally more efficient in some cases. This implementation forms a multiscale basis, containing individual flux responses for mortar degrees of freedom. Next we apply this discretization to the stochastic collocation method for uncertainty quantification of flow in porous media. The governing equations are based on Darcy's law with stochastic permeability represented as a Karhunen-Loeve (KL) expansion. We consider a non-stationary case, in which there are multiple KL expansions modeling different rock types. We show how the multiscale flux basis implementation can be used to make this algorithm computationally more efficient by several orders of magnitude.

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**MS9**

**Finite Element Approximation of Time Dependent Stokes Darcy Interface Problems**

We use the time dependent Stokes-Darcy model to characterize fluid flow in karst aquifers. The full form of Beavers-Joseph interface condition is used instead of the simplified Beavers-Joseph-Saffman condition. Convergence and error estimates for the finite element approximations are obtained and is verified by numerical experiments. The results from the flow simulation are used to study transportation of contaminants in the karst aquifer. These numerical simulations are qualitatively compared with the laboratory experiments.

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**MS9**

**On the Equation of Poroelasticity**

The theory of porelasticity describes the mechanical behavior of elastic porous media and in particular, the elastic behavior (the swelling and shrinking) of fluid-saturated porous media. Electro-poroelasticity also allows for the interaction of the fluid-saturated porous media with electromagnetic fields. Many natural substances, e.g., rocks, soils, and biological tissues, as well as man made materials such as foams, gels, concrete, and ceramics can be considered as elastic porous media. Thus poroelasticity models

which were originally developed in the context of geomechanics and rock mechanics find applications in a multitude of areas. In this talk I will illustrate some of the properties of the equations of quasi-static poroelasticity and electroporoelasticity, and describe some numerical methods for approximating their solutions.

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**MS9**
**Numerical Methods for Stokes Equations**

This talk will focus on domain decomposition and multilevel methods for Stokes equations. The goal is to investigate the convergence for these methods when directly applied to the saddle point problem.

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**MS10**
**Efficient Calculation of Pareto-optimal Points in Aerodynamic Shape Optimization**

The talk concerns the development of mathematical methods, algorithmic techniques and software tools for the transition from simulation to optimization. The methodology is applicable to all areas of scientific computing, where large scale governing equations involving discretized PDEs are treated by custom made fixed point solvers. To exploit the domain specific experience and expertise invested in these simulation tools we propose to extend them in a semi-automated fashion. First they are augmented with an adjoint solver to obtain (reduced) derivatives and then this sensitivity information is immediately used to determine optimization corrections. In other words, rather than applying an outer optimization loop we prefer the 'one-shot' strategy of pursuing optimality simultaneously with the goals of primal and adjoint feasibility. Finally, we discuss how to use these methodologies in order to calculate pareto-optimal points in aerodynamic shape optimization for robust designs.

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**MS10**
**Shape and Topological Optimization under Uncertainty**

For deterministic shape optimization of elastic structures we present a level set method that incorporates efficient solution of elasticity PDEs. Combining shape and topological derivatives improves the optimization and avoids bad local minima. Additional morphological smoothing operations facilitate the numerical treatment of elasticity PDEs. Shape optimization of elastic structures under random volume and surface forces is done in a framework inspired by two-stage stochastic programming. Our first formulation of stochastic shape optimization aims at finding a shape minimizing the expected value of the shape objective functional. We extend the stochastic optimization perspective by considering risk measures. In particular, these are the expected excess and the excess probability.

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**MS10**
**Robust Shape Optimization in CFD**

Recently, optimization has become an integral part of the aerodynamic design process chain. However, because of uncertainties with respect to the flight conditions and geometry uncertainties, a design optimized by a traditional design optimization method seeking only optimality may not achieve its expected performance. Robust optimization deals with optimal designs, which are robust with respect to small (or even large) perturbations of the optimization setpoint conditions. That means, the optimal designs computed should still be good designs, even if the input parameters for the optimization problem formulation are changed by a non-negligible amount. Thus even more experimental or numerical effort can be saved. In this talk, we aim at an improvement of existing simulation and optimization technology, so that numerical uncertainties are identified, quantized and included in the overall optimization procedure, thus making robust design in this sense possible. Beside the scalar valued uncertainties in the flight conditions we consider the shape itself as an uncertainty source and apply a Karhunen-Loeve expansion to approximate the infinite-dimensional probability space. To overcome the curse of dimensionality an adaptively refined sparse grid is used in order to compute statistics of the solution. These investigations are part of the current German research program MUNA.

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**MS10**
**Non-parametric Shape Optimization in CFD**

In aerodynamic shape optimization and elsewhere it is often claimed that the adjoint approach makes the computation of the gradient independent of the number of un-

knowns. However, the need to compute so called "mesh sensitivities' in practical applications has so far proven to be a major obstacle to an industry size large scale aerodynamic shape optimization. As a remedy, we present shape calculus techniques which result in a shape derivative that exists only on the surface of the aircraft and can be computed without any sensitivities at all. By staying in the analytical framework all the time, we arrive at a gradient formulation which is independent of any parameterization like free-form, b-splines, or CAD. Thus, a large deformation of the shape is possible while the gradient is still very cheap to compute. The resulting loss of regularity is treated by considering the shape Hessian, which is derived for a Stokes flow. We also show shape Hessian approximations for the Navier-Stokes and Euler equations using operator symbols.

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**MS11**

**Multiple Scale Modeling using Scale Relative Geometries**

Scale variant behavior of a phenomenon is related to variations in local curvature of the manifold on which the dynamics exist. Nonlinear associative effects like memory are realized via changes of curvature as the system evolves. Model equations on these manifolds maintain their form across scales allowing one to seamlessly move across scales. In this talk I would present the foundations of these ideas, related geometrical calculus and concepts useful for developing computer simulations.

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**MS11**

**Multilevel Modeling in Highly Heterogeneous Media**

Multilevel upscaling of single-phase saturated flow is presented that explicitly creates the coarse-scale model through the operator-induced variational coarsening of the fine-scale model. In this talk we highlight the flexibility and features of this approach for diffusive models, such as single-phase Darcy flow and simplified two-phase flows. In addition, we will discuss its potential application to models with advection, such as the advection-dispersion-reaction equation.

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**MS11**

**Bridging Scales: A Three-dimensional Electromechanical Finite Element Model of Skeletal Muscle**

The emphasis of this talk will be on the electromechanical coupling of electrophysiological properties and the biomechanical response of the whole muscle. To bridge the spatial scales between cellular and the whole organ level, homogenized values of key physiological parameters, e.g. the pre- and post-power stroke concentration of crossbridge attachments, are incorporated within a macroscopic constitutive law of skeletal muscle tissue. A convergence study comparing the electromechanical model with a mechanical-only model is presented.

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**MS11**

**Multilevel Hierarchies of Models for Two-Phase Flows in Porous Media**

Flow simulations in porous media formations involve a wide range of strongly coupled scales. In modeling single and two-phase flow in porous media the strongest multiscale influence arises from the heterogeneous structure of the subsurface environment. The permeability of rock formations is highly heterogeneous and may span several orders of magnitude, from nearly impermeable barriers to high-permeable flow channels. For such complex systems fully resolved simulations become computationally intractable. The goal of multiscale modeling is to developed methods

which upscale fine-scale model, not just its parameters. In our work we propose the new Multilevel Multiscale Mimetic method ($M^3$). This approach brings together a subgrid modeling algorithm for developing mimetic discretizations on coarse scales proposed by Yu. Kuznetsov with algebraic multigrid for estimating moments of the flux on the edges. Multilevel hierarchy of coarse scale discretizations makes it very flexible and computationally efficient. Due to the algebraic nature of the method it can be naturally adopted to the different types of fine scale discretization, such as: Mixed Finite Element method, Finite Volume method, Mimetic Finite Difference method. Moreover the method can handle full permeability tensor and general types of fine and coarse scale partitions.

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**MS12**

**DoD CREATE Air Vehicle program**

An overview of the CREATE program for developing a simulation capability for Air Vehicles will be discussed.

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**MS12**

**Designing Adaptive Mesh Simulators for Reacting Flows Using the Common Component Architecture**

Direct numerical simulations of reacting flows are often conducted using the low-Mach approximation of the Navier-Stokes equations, solved on adaptively refined meshes, with custom-designed integration and projection schemes. In our talk we will describe how multiple third-party libraries were integrated via the Common Component Architecture to construct a toolkit for simulating flames. We will present simulation results and discuss metrics to quantify the reduction of software complexity effected by adopting a component-based paradigm.

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**MS12**

**Building Production PDE Applications from Trilinos Components**

I will discuss our vision for being able to rapidly build new production PDE codes with transformational analysis capabilities, and our current state of progress towards that vision. The first part of the plan is to create a full buffet of independent software packages – with capabilities ranging from preconditioners to finite element libraries to UQ algorithms – that are delivered, compiled, and tested as part of Sandia's Trilinos framework. The second part is to build driver applications that push interoperability, the development of abstract interfaces, sophisticated use-cases, and mature software quality environmnets.

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**MS12**

**Multi-Physics Software Engineering with Uncertainty Quantification**

In this presentation, we present an overview of the PECOS Center effort to develop a next-generation computational method for modeling reentry vehicles into the atmosphere with formal modeling uncertainty quantification (UQ) included. In this effort, we document some of the challenges faced in a large-scale scientific software development project that arise when coupling individual physical models written in multiple languages, with potentially disparate length/time scales and alternate dimensionalities (models include high-speed flow, radiation, chemistry, and ablation).

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**MS13**

**Towards Shape Optimization for Ventricular Assist Devices Using Parallel Stabilized FEM**

Several challenges and methods in biomedical flow device design are described. The objective often involves the unique behavior of blood as the flowing medium, necessitating, e.g., accurate modeling of thrombosis and hemolysis. The fluid constitutive behavior, in particular shear-thinning, may affect the outcome of shape optimization more than it affects direct flow analysis. Finally, target applications often involve intricate time-varying geometry, and thus, realistic solutions can be only obtained on high-performance parallel computers.

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**MS13**

**Electrical and Mechanical Problems in Cardiovascular Modelling**

We address various issues related to fluid-structure interaction in the cardiovascular system and on the electrical activity of the heart. We will focus on the cardiac valves simulation, including the management of contact between leaflets, and on the electro-mechanical coupling in the myocardium.

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**MS13**

**An Efficient Preconditioner for the Bidomain Model in Electrocardiology**

We present a preconditioner for the Bidomain system governing the propagation of action potentials in myocardial tissue. The degenerate nature of the problem results in a severe ill conditioning of its discretization. Our preconditioning strategy is based on an adaptation of the Monodomain model, which is simpler to solve, nevertheless is unable to capture significant features of the solution. We prove optimality for the preconditioner, and corroborate results with numerical simulations in real geometries.

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**MS13**

**Mathematical Models and Numerical Approximation of Controlled Drug Release from Stents**

A stent is a small mesh tube inserted permanently into a stenotic artery. The design of such devices is a complex task because their performance is affected by the geometrical design, the mechanical properties of the materials and the chemical properties of the drug. Mathematical models and numerical simulation techniques are appropriate to study such phenomena with the aim to be used as a predictive tool for the design of optimal drug eluting stents.

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**MS14**

**Total of Eight Student Speakers (four in each session) To Be Announced January 2009**

Abstract not available at time of publication.

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**MS15**

**Adaptive Finite Element Methods for Flow Problems**

The accurate simulation of the unsteady Navier-Stokes equations is still a major challenge for science and engineering. In this talk we present the basic theory and evaluate some numerics for adaptive finite element methods based on a posteriori error estimates and duality. We experiment with different goals of the overall computation and discuss the qualitative behavior of a linearized dual solution. We also touch upon the question of which flow quantities (e.g., drag, vorticity, point values of velocity) can be computed and not. We do this using numerical experiments computed in parallel with a Standard Upwind Petrov Galerkin method in combination with the variational multiscale method, and weak Nietsche type boundary conditions.

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**MS15**

**Recent Developments for A Posteriori Error Estimation and Adaptive Error Control for Evolution Problems**

Significant problems face the use of adaptive discretization for evolution problems, including global error control of quantities of interest, accounting for cancellation of error and changing stability, and dealing with the affects of mesh refinement on accuracy and stability. We describe recent work addressing these issues. This work includes a probabilistic framework replacing the standard optimization framework, a blockwise-adaptive parallel-efficient adaptive strategy, and the effective use of coarse scale adjoint information for error estimation, especially in employing the adjoint to drive compensated domain decomposition, a new framework for multiscale time integration.

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**MS15**

**Application of Adaptive Discontinuous Galerkin Methods to Bifurcation Phenomena in Pipe Flows**

In the past, studies of bifurcation phenomena of flow in

a cylindrical pipe with a sudden expansion have proven inconclusive. In this work we seek to exploit the O(2)-symmetric properties of the problem, thus making it tractable by reducing the underlying three-dimensional problem to a series of two-dimensional ones. For the numerical solution of the Navier-Stokes equations we employ an interior penalty Discontinuous Galerkin method, together with goal-oriented error estimation techniques to guarantee the accurate identification of bifurcation points.

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**MS15**

**Adaptive Finite Element Methods for Eigenvalue Problems with Applications in Model Reduction**

Linear elastic eigenvalue problems are one of the most common applications of finite element methods in industry. In this talk we present an adaptive finite element method based on a posteriori error estimates for such problems and we consider several applications to real three dimensional mechanical components. We emphasize, in particular, problems with multiple eigenvalues. Finally, we discuss adaptive model reduction algorithms for mechanical components that build on certain multilevel eigenfunction expansions.

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**MS16**

**Computational Science and Engineering at San Diego State University**

The computational science graduate program at san diego state's CSRC is a novel educational initiative. The aim of the program is to educate professional researchers capable of effectively utilizing modern computational tools to tackle a variety of cutting-edge scientific problems. The distinctive feature of the program is its interdisciplinary character; even though the program is driven by the science computation as a fundamental tool is emphasized as the program exposes students to a broad cross section of the applied sciences. The CSRC achieves its interdisciplinary status by partnering students with courses and professors from the applied sciences: biology, chemistry, computer science, engineering, geology, mathematics, and physics. the computational science students pursue coursework and research from this wide range of disciplines. Our PhD program has been ranked in the top 10 nationwide by Academic Analytic.

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**MS16**

**The 2009 Krell Institute Survey of Computational Science and Engineering Education Programs**

Since 1992, the author has maintained a survey of computational science and engineering (CSE) courses and programs. The 2009 version includes detailed information on approximately one hundred undergraduate and graduate programs in the United States. We will discuss trends revealed by the survey, including the core CSE courses in the curriculum, the prominence of major versus minor or emphasis programs, CSE in liberal arts and community colleges, and the role of high performance computing.

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**MS16**

**A Blank Slate: Building a New Computational Science Program at a New University**

Efforts at many universities to build programs in computational science run into difficulties associated with fitting a new interdisciplinary curriculum within the confines of many well-established, mature and predominantly single-disciplinary programs. University of California in Merced (UCM) is a brand new university which was built with a focus on interdisciplinary research. UCM is undergoing development and growth unprecedented for many other schools. Building a CSE program at UC Merced offers an opportunity to investigate what would be essential components of an effective program if it has to be built from scratch with much fewer academic institutional constraints than at other universities. In this talk we will discuss efforts and challenges in integrating CSE into the curriculum and degree programs at UCM.

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**MS16**

**UTEP Computational Science Program**

Computational Science is an interdisciplinary program, crossing departmental and college boundaries, that yields an integrated knowledge-base for the effective solution of complex problems where computer usage plays a fundamental role. UTEP offers studies leading to degrees of a Doctor of Philosophy and Master of Science in Computational Science. During this talk, the program and its opportunities for creating a new generation of computational scientists will be described.

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**MS17**

**High-Order Methods for Ocean Modeling**

Numerical ocean models based on unstructured meshes have been under intensive development for the past decade. There is a considerable effort in using high-order methods for ocean modeling. High-order methods offer the promise of accurately capturing the oceanic processes and have been shown to efficiently scale to large number of processors. In this talk, I would discuss the advantages and disadvantages of high-order methods, in particular discontinuous Galerkin method for ocean modeling using the unstructured mesh generated by centroidal Voronoi tessel-

lations.

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**MS17**

**A Specialized Parallel Elliptic Solver for Thin Aspect Ratio Domains: The Rectangular Case**

The simulation of stratified oceanic turbulence is quite challenging since it exhibits a very large scale spectrum, and occurs in thin aspect ration domain whose horizontal extent is much larger then its vertical one. Here we exploit this geometric disparity to design a scalable parallel iterative solver tailored for this kind of geometry. The aim is to improve our capability to simulate oceanic turbulence at high Reynolds and Prandtl numbers using non-hydrostatic oceanic models. The solver is based on a combination of domain decomposition techniques and fast fourier solvers. Its performance within the context of a spectral element discretization will be presented and contrasted to the performance of other iterative based solvers.

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**MS17**

**A Multi-resolution Method for Climate System Modeling**

During the next decade and beyond, climate system models will be challenged to resolve scales and processes that are far beyond their current scope. Each climate system component has its prototypical example of an unresolved process that may strongly influence the global climate system. These new demands will almost certainly result in the develop of multi-resolution schemes that are able, at least regionally, to faithfully simulate these fine-scale processes. Spherical Centroidal Voronoi Tessellations (SCVTs) offer one potential path toward the development of robust, multi-resolution climate system model component. SCVTs allow for the generation of high quality Voronoi diagrams and Delaunay triangulations through the use of an intuitive, user-defined density function. Real-world examples are developed for the Greenland ice sheet and the North Atlantic ocean. Idealized examples are developed for ocean-ice shelf interaction and for regional atmospheric modeling. In addition to defining, developing and exhibiting SCVTs, we pair this mesh generation technique with a previously developed finite-volume method. Our numerical example is based on the nonlinear shallow-water equations spanning the entire surface of the sphere and is used to elucidate both the potential benefits of this multi-resolution method and the challenges ahead.

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**MS17**

**Approximating Stationary Statistical Properties of Infinite Dimensional Dissipative Dynamical Systems**

Computing the long time behavior such as the climate or stationary statistical properties of large complex systems has been a long standing challenge. We present a general result indicating that certain numerical schemes are able to capture the climate (stationary statistical properties) of infinite dimensional dissipative dynamical systems. Application to the infinite Prandtl number model will be discussed as well.

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**MS18**

**Blood Flow Models and Their Application to Cardiovascular Diseases**

We provide an overview of multi-scale mathematical modeling efforts focused on understanding cardiovascular disease development and treatment. Using modeling and simulation, we demonstrate how to provide insight into disease development and effects of compound intervention. We provide an example that demonstrates the use of modeling in understanding how changes in the properties of some vascular beds may affect biomarkers of disease. This analysis aids in design of experiments and development of better biomarkers for profiling the hemodynamic fingerprint of a compound in development.

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**MS18**

**Variational Multiscale Modeling for Drug Delivery**

A variational framework for modeling non-linear multiphysics problems is presented for standard and isogeometric finite element methods. The variational formulation is designed such that fundamental mathematical and physical features of the solution are built into the weak form, while the formulation is kept flexible and robust. The construction of the variational form is twofold. First, a multiscale decomposition of the solution into coarse and fine scales is introduced a priori. The coarse scales are identified with the finite element approximation, while the fine scales are identified with the subgrid scales and need to be modeled. Using the Navier-Stokes equations as a model problem, a residual-based approximation of the fine scales is made. Second, weak imposition of boundary conditions and coupling is used to introduce physical modeling when necessary. This presentation will discuss the variational framework used to model drug delivery in idealized and patient-specific geometrical models of the cardiovascular system, where the variational multiscale method is used to stabilize the weak form and weak imposition of boundary conditions is used to model endothelial permeability, In ad-

dition, an adhesion model for suspended nanoparticles will be presented. NURBS-based isogeometric analysis is employed to describe the geometry and discretize the balance equations.

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**MS18**

**Multiscale Modeling of Intravascular Nano-particle Cancer Drug Delivery**

The focus on the talk will be a problem motivated by cancer drug delivery using nano-particles, brought to our attention by Mauro Ferrari, the Director of the Center for Nano-Medicine at the UT Health Science Center in Houston. The main goal is to understand how pulsation of arteries influences dispersion of nanovectors used for intravascular delivery of drugs and contrast agents. The mathematical problem is that of Taylor dispersion in small channels with compliant walls. We used and developed novel mathematical and computational techniques to study advection and diffusion of passive tracers (nano-particles) in domains with a moving boundary. The results are interesing: pulsation of arterial walls enhances the probability for nanoparticle wall adhesion and uptake by the diseased tissue. The mathematical model, computations and movies showing the results will be discussed.

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**MS18**

**Modelling Transport Phenomena in the Arterial Wall with Application to Drug Eluting Stent**

Stents are medical devices used to cure stenosis, typically in coronaries. In the last years a new type of stents have been devised where a thin polimeric coating filled with appropriate drugs is placed on the stent stucture. A controlled release of the drug into the vessel wall may reduce inflammatory processes and the risk of restenosis. In this work we will present some mathematical and numerical methods to simulate the release process and estimate the efficacity of the drug.

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**MS19**

**Dynamics of Erythrocytes in Strong Flows via a Three-dimensional Interfacial Spectral Boundary Element Algorithm**

The study of the interfacial dynamics of artificial or physiological capsules (i.e. membrane-enclosed fluid volumes) in Stokes flow has seen an increased interest during the last few decades due to their numerous engineering and biomedical applications. However, the computational study of the capsule dynamics at high flow rates is limited owing to the coupling of the fluid dynamics with the membrane elastic-solid properties. To overcome this, we have developed a spectral boundary element algorithm for interfacial dynamics of three-dimensional capsules in Stokes flow. Our methodology preserves the main characteristic of the spectral methods, i.e. the exponential convergence in the interfacial accuracy as the number of spectral points increases, but without creating denser systems as spectral methods used in volume discretization do. Owing to its spectral nature, our interfacial algorithm has the significant advantage of the accurate determination of any interfacial property, including geometric derivatives and membrane tensions. We believe that this is an important issue for the correct and accurate determination of very deformed capsule shapes made from membranes obeying non-linear elastic laws. To investigate the erythrocyte dynamics in strong shear flows, we employ our interfacial spectral boundary element algorithm properly extended to model the erythrocyte's biconcave disc reference shape and surface-area incompressibility. Our computational results for the cell deformation are in excellent agreement with experimental findings from ektacytometry. In addition, our computational work allows analysis of the erythrocyte dynamics beyond the capabilities of ektacytometry and other experimental techniques which see the cell from one view-angle only. In this talk I will discuss the swinging motion of the erythrocytes observed at high shear rates and how it is affected by the flow rate and the viscosity ratio. My talk also includes our recent results on the hemopathology in the microcirculation.

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**MS19**

**A Velocity Decomposition Approach for Moving**

**Interfaces in Viscous Fluids**

We present a second-order accurate method for computing the coupled motion of a viscous fluid and an elastic material interface with zero thickness. The fluid flow is described by the Navier-Stokes equations, with a singular force due to the stretching of the moving interface. We decompose the velocity into a "Stokes" part and a "regular" part. The first part is determined by the Stokes equations and the singular interfacial force. The Stokes solution is obtained using the immersed interface method, which gives second-order accurate values by incorporating known jumps for the solution and its derivatives into a finite difference method. The regular part of the velocity is given by the Navier-Stokes equations with a body force resulting from the Stokes part. The regular velocity is obtained using a time-stepping method that combines the semi-Lagrangian method with the backward difference formula. Because the body force is continuous, jump conditions are not necessary. For problems with stiff boundary forces, the decomposition approach can be combined with fractional time-stepping, using a smaller time step to advance the interface quickly by Stokes flow, with the velocity computed using boundary integrals. The small time steps maintain numerical stability, while the overall solution is updated on a larger time step to reduce computational cost.

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**MS19**

**Multipole-accelerated Calculations of Emulsion Flow through a Granular Material**

A novel multipole-accelerated boundary-integral algorithm is used for large-scale simulations of many deformable drops flowing through a packed granular material. Solid frictional particles form a random mechanically-equilibrium contact network with 50-55% density. Non-deformed drop radius is larger than the pores, squeezing meets high resistance necessitating superhigh resolution ( 10000 boundary elements per surface). Drop and continuous-phase permeabilities are studied, including ensemble averaging, critical squeezing conditions and multiple drop breakup.

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**MS20**

**Partitioning Sparse Matrices**

Matrix partitioning is an important technique for enabling inherent parallelization in solvers for mathematical programming, $LU$ factorization and $QR$ factorization, for improving performance of parallel sparse matrix vector multiplications, and for finding fill-reducing orderings via nested disection. During the last decade, several, successful hypergraph-based models and methods are proposed for matrix partitioning. In this talk, we will comparatively review those models and methods.

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**MS20**

**Parallel Sparse Matrix Ordering with Zoltan**

The performance of sparse direct solvers is sensitive to the ordering of the input matrix. Therefore, much attention has been given to methods that orders the matrix to minimize the number of operations required by the factorization. Nested dissection is the preferred method for large problems, however, most available tools are designed for symmetric matrices. Zoltan and Isorropia provide a standardized way for parallel sparse matrix ordering, by using existing tools for symmetric cases. We discuss a parallel implementation of the HUND algorithm for nonsymmetric problems in progress, based on Zoltan's hypergraph partitioner. We show preliminary experiments on large matrices.

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**MS20**

**Multifrontal Multithreaded Rank-revealing Sparse QR Factorization**

SuiteSparseQR is a sparse QR factorization package based on the multifrontal method. Within each frontal matrix, LAPACK and the multithreaded BLAS enable the method to obtain high performance on multicore architectures. Parallelism across different frontal matrices is handled with Intel's Threading Building Blocks library. The symbolic analysis and ordering phase pre-eliminates singletons by permuting the input matrix into the form $[R_{11}\, R_{12}\, ;\, 0\, A_{22}]$ where $R_{11}$ is upper triangular with diagonal entries above a given tolerance. Next, the fill-reducing ordering, column elimination tree, and frontal matrix structures are found without requiring the formation of the pattern of $A^T A$. Rank-detection is performed within each frontal matrix using Heath's method, which does not require column pivoting. The resulting sparse QR factorization obtains a substantial fraction of the theoretical peak performance of a multicore computer.

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**MS20**

**Solving Linear Systems For Multiple Sparse Right-**

**Hand Side Vectors in Out-of-Core Environment**

We consider the solution phase of multifrontal solvers for sparse right-hand side vectors in an out-of-core context, where factors of the frontal matrices are stored on disk. In this framework, the loading of the factors is the most consuming time operation. For applications that use the solution phase intensively, it is necessary to minimize the cost associated with this operation. We will describe the problem formally and investigate possible solutions.
Key words: sparse right-hand side, direct methods, multifrontal solver, LU factorization.

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**MS21**

**Lattice Boltzmann Simulation on GPUs - An Approach to Grid Refinement**

In this talk we will present different approaches to grid refinement for lattice Boltzmann methods using graphics processing unit (GPU) hardware. The programming model and especially the data access and processing are for GPUs quite different from those of CPUs and therefore suitable algorithms for grid refinement have to be developed. We will present and discuss the advantages and drawbacks of different approaches.

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**MS21**

**Lattice-Boltzmann Simulation of Thermal Flows Induced by Radiative Heat Transfer**

In this talk we will present a coupling approach for the simulation of turbulent flows induced by radiative heat interacting with solid boundaries interacting with a fluid. We will demonstrate the feasibility of the approach for various engineering applications related to building climate comfort modeling.

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**MS21**

**Direct Numerical Simulation of Isotropic Turbulence by Using the Lattice Boltzmann Equation**

We compare the lattice Boltzmann equation (LBE) and the pseudo-spectral (PS) methods for DNS of the decaying isotropic turbulence in a 3D periodic cube. We use a mesh size of $N^3 = 128^3$ and the Taylor micro-scale Reynolds number $24.35 \leq \mathrm{Re}_\lambda \leq 72.37$, and $t \approx 30\tau_0$, where $\tau_0$ is the turbulence turnover time. Our results indicate that the resolution requirement for the LBE is $\delta x/\eta_0 \leq 1.0$, approximately twice of the requirement for PS methods, where $\delta x$ and $\eta_0$ are the grid spacing and the initial Kolmogorov length. The LBE is shown to be a reliable and accurate method for the DNS of decaying turbulence.

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**MS21**

**Lattice-Boltzmann-based Large-eddy Simulation: Advanced Modelling Approaches**

This talk adresses the development of advanced subgrid model for large-eddy simulations (LES) of turbulent flows based on Lattice-Boltzmann methods (LBM). Most existing subgrid closures used in LES-LBM are nothing but straightforward extensions of the crudest model developed within the Navier-Stokes framework, namely the Smagorinsky eddy-viscosity model. In a first part, it will be shown how to obtain an improved eddy-viscosity subgrid model for LBM. The original implementation of the Inertial-Range Consistent Smagorinsky model proposed by Dong

and Sagaut (2008) for the D3Q19 scheme will be used as an illustration. In a second step, an original extension of the Approximate Deconvolution Method proposed by Adams and Stolz for Navier-Stokes simulation will be considered. This new LBM-LES approach doesn't rely on the eddy-viscosity concept and is written directly within the LBM framework. It can be implemented thanks to a trivial modification of existing LBM solvers for Direct Numerical Simulation.

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**MS22**

**Utilizing Sparsity Patterns in SVM Kernels**

Support Vector Machine (SVM) is concerned with obtaining maximum-margin hyperplanes over a set of points in a d-dimensional space. The separating hyperplane is the one that maximizes the distance from the nearest datapoint. The set of data points are represented as a matrix and in many applications, such as textmining, this matrix is sparse. In this presentation we examine how the sparsity pattern can be exploited to improve the efficiency of SVM.

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**MS22**

**ParaText: Leveraging Scalable Scientific Computing Capabilities for Large-Scale Text Analysis and Visualization**

ParaText is a text analysis engine for processing and searching large collections of documents. The retrieval method employed in ParaText is latent semantic analysis, in which a matrix SVD is used. In this talk, we demonstrate the use of ParaText in a fully scalable text analysis pipeline, which leverages the distributed memory capabilities of the Trilinos and ParaView frameworks originally developed for distributed linear algebra and visualization support in scientific computing applications.

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**MS22**

**Homotopy Continuation Methods for Clustering Relational Schemas**

Clustering relational schemas is an important problem with applications in cross-genomic studies, information retrieval, and temporal data mining. The key idea in this talk is to mirror the schema of the relational database in the structure of the clustering objective function. We show how our framework generalizes the goals of many different clustering formulations and also enables the use of homotopy continuation methods to reason about how different data sources can be systematically combined.

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**MS22**

**Toward a Programming Model for Data Analysis and Mining**

The goal of the Tree-based High-Order Reduce (THOR) project is to develop a new domain-specific programming model that permits rapid automatic implementation of customized parallel statistical data analysis and mining tasks with minimal coding effort. In this talk, we outline how the underlying mathematical formalism, called the generalized n-body problem (GNP) theory (developed by Gray), enables the development of a program generator and tuning framework for parallelized GNP solvers.

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**MS23**

**Fluid-structure Interaction in Blood Flow: Analysis and Numerics**

The focus of this talk will be on the analysis and computation of fluid-structure interaction in blood flow. Understanding solutions to moving-boundary problems describing fluid-structure interaction between blood flow and arterial walls is important in understanding the mechanisms leading to various complications in cardiovascular function. Although fascinating progress has been made in some areas of modeling and simulation of the human cardiovascular system many of the basic difficulties remain open and will continue to present major challenges in the years to come. The speaker will give an overview of the main problems and difficulties associated with the study of fluid-structure interaction in blood flow. Recent results in the analysis of solutions to the benchmark problem in blood flow, obtained by the group at the University of Houston, will be summarized and recent developments in the numerical algorithm design will be mentioned. Applications involving certain cardiovascular applications will be shown. Colalborators: Dr. Z. Krajcer and Dr. D. Rosenstrauch (Texas Heart Institute), Dr. C. Hartley (Baylor College of Medicine), Prof.

R. Glowinski, Prof. T.W. Pan, Prof. G. Guidoboni (University of Houston), Prof. A. Mikelic (University of Lyon 1, FR), Prof. J. Tambaca (University of Zagreb, CRO)

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**MS23**

**Verification Study of the Coupled Momentum Method for Modeling Blood Flow in Compliant Arteries Using Womersleys Deformable Wall Analytical Solution**

In this work, we perform the verification study of the mathematical model for blood flow in compliant arteries given by the Coupled Momentum method (Figueroa, 2006). The verification of this model is done using Womersleys deformable wall analytical solution for pulsatile flow in a semi-infinite cylindrical vessel. This solution is, under certain premises, the analytical solution of the Coupled Momentum method.

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**MS23**

**Unsteady 3D Flow Simulations in Cranial Arterial Tree**

Two-level domain partitioning and Multi-level Communicating Interface have been developed for large scale 3D arterial flow simulation on petascale computes. We present an implementation of the new numerical methods for high-resolution simulation of an unsteady flow in arteries of the human brain. Solution of 2.8 billion degrees of freedom problem defined in a domain of 147 arteries discretized into 1,244,295 high-order spectral elements was obtained in 1.1 sec per time step on 18,576 processors.

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**MS23**

**CFD/MRI-Based Functional Imaging in Arteries**

A specific phase-locked MRI protocol is used in order to extract the full geometry of arterial sectors at several phases over the cardiac cycle. These data are the input of a dedicated CFD code for the computation of the corresponding blood flow response with actual hemodynamic conditions and unsteady geometry. Some of the challenges which must be addressed before this CFD/MRI-based functional imaging technique can be used in the clinical routine are discussed.

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**MS24**

**Total of Eight Student Speakers (four in each session) To Be Announced January 2009**

Abstract not available at time of publication.

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**MS25**

**Adaptive Finite Element Methods for Inverse Imaging Problems**

In many realistic 3d imaging problems, such as tumor diagnostics, the resolution requested by practitioners is unachiavable using globally refined meshes. However, while now the leading paradigm in PDE solvers, adaptivity has not been widely used for inverse problems. We will present a mathematical framework for imaging applications using automatically adapted meshes, and present results obtained for three-dimensional optical tomography for tumor detection using multiple measurements obtained when illuminating a body with different light patterns.

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**MS25**

**Adaptive Variational Multiscale Methods with Applications in Oil Reservoir Simulation**

We present a mixed adaptive variational multiscale method for solving elliptic second order problems. The method is based on a particular splitting into coarse and fine scales together with a systematic technique for approximation of the fine scale part based on solution of decoupled localized subgrid problems. We also present an a posteriori error estimate and an adaptive algorithm, based on the estimate. Finally, we present numerical examples with data from a model oil reservoir.

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**MS25**

**Goal Oriented Adaptivity for the Control of Modeling Errors in Multiscale Simulations**

We will present recent progress on the development of an adaptive strategy for the control of modeling error in atomic-to-continuum coupled simulations. The method is based on the Arlequin framework that introduces an overlap region to couple the continuum and molecular models. A goal-oriented adaptive strategy is used in order to determine the optimal position of the overlap so as to reduce the modeling errors in quantities of interests within preset levels of accuracy.

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**MS25**

**Adjoint Based Optimization and Adaptivity for Flow and Transport Problems**

We present an adjoint based approach to improve the accuracy of large scale flow and transport problems using adaptivity. Stabilized finite element are investigated for the convective dominated dynamics. Interesting challenges arise in the adjoint calculation and the associated error estimator. We present numerical tests to verify our approach in addition to applying our techniques to large scale applications and optimization problems.

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**MS26**

**Efficient Methods for Solving Separable Nonlinear Inverse Problems arising in Medical Imaging Applications**

Ill-posed inverse problems arise in many engineering applications, and oftentimes the model for the problem is nonlinear and depends on various parameters which can only be obtained approximately. We consider efficient iterative approaches to solve separable nonlinear least squares problems, specifically for large scale inverse problems. A variable projection Gauss-Newton method is used to solve the nonlinear least squares problem, and Tikhonov regularization is incorporated using an iterative Lanczos hybrid scheme. We discuss a nonlinear solver that requires very little input from the user and illustrate its effectiveness in medical imaging simulations.

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**MS26**

**Increasing Living Kidney Donation with Optimization; Influencing Public Policy with Simulation**

Kidney paired donation matches a patient and incompatible donor with another patient and donor for an organ exchange. Barriers; political, ethical, and technical, are addressed using CSE tools. Simulations demonstrating paired donation's impact on the kidney shortage motivated Congressional action. Letting patient-donor pairs be vertices of a graph, with an edge between two vertices if a paired donation is possible, we select a largest set of donations using weighted graph matching algorithms.

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**MS26**

**Accurate Molecular Properties Using a Massively-Parallel Quantum Chemistry Code and Implications for Drug Design**

The development of computationally inexpensive yet accurate models for evaluating pharmaceutical activity of potential drugs is an extremely important application in computational chemistry relevant to both academic and industrial researchers. I will outline a solution to some of the challenges of developing these models which uses quantum chemical data sets to produce accurate general purpose models. The massively-parallel implementation of coupled-cluster response theory within NWChem, which makes this task possible, will be discussed.

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**MS26**
**Lighting up Dark Matter and Dark Energy Through Large-scale Simulation**

As major new observatories, such as the Dark Energy Survey, come online, there is an intense need to directly link what we can see stars, galaxies, diffuse x-rays, radio emissions, etc. to what we can't dark matter and dark energy. I will discuss how large-scale multiphysics simulations of cluster of galaxies (the largest gravitationally-bound objects in the universe) bridge that essential gap, allowing us to peer into the heart of dark matter structures, divine the role that dark energy plays in our universe, and provide a gateway to studying the long-term evolution of the cosmos as a whole.

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**MS27**
**Is The Choice of Ocean Vertical Coordinate of Importance in Climate Modeling?**

The choice of vertical coordinates in ocean models has a strong impact on the resulting ocean circulation, in large part because of the representation of unresolved physics. This presentation will give a brief overview of the vertical coordinates currently used in ocean models and then discuss the behavior of two ocean models currently used in the CCSM framework when forced with identical atmospheric fields.

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**MS27**
**Geoengineering by Seeding Boundary Layer Clouds Using Two Climate Modeling Paradigms**

We explore the Earth system climate response to geoengineering by seeding maritime boundary layer clouds. We contrast the response of the system using an atmospheric GCM coupled to two different formulations for sea ice and ocean dynamics: 1) a full ocean and dynamic sea ice model; 2) a slab ocean model with a thermodynamic sea ice model. We show that the climate response is quite different in the two formulations and explore the reason for the difference.

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**MS27**
**On the Stochastic Primitive Equations of the Ocean**

The primitive equations of the ocean are the Navier-Stokes equations considered on a thin domain with a rotational Coriolis term. We consider the existence and uniqueness of two-dimensional such flows with an additive Gaussian forcing on a periodic domain. We also look at some probabilistic properties of the resulting solutions.

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**MS27**
**Reconciling non-Gaussian Atmosphere-Ocean Statistics with Linear Dynamics**

Linear stochastically forced models have been found to be competitive with comprehensive nonlinear weather and climate models at representing many features of the observed covariance statistics and at predictions beyond a week. Their success seems at odds with the fact that the observed statistics can be significantly non-Gaussian, which is often attributed to nonlinear dynamics. The stochastic noise in the linear models can be a mixture of stateindependent ("additive") and linearly state-dependent (multiplicative") Gaussian white noises. It is shown here that such mixtures can produce not only symmetric but also skewed non-Gaussian probability distributions if the additive and multiplicative noises are correlated. Such correlations are readily anticipated from first principles. A generic stochastically generated skewed (SGS) distribution can be analytically derived from the Fokker-Planck equation for a single-component system. In addition to skew, all such SGS distributions have power-law tails, and a striking property that the (excess) kurtosis K is always greater than 1.5 times the square of the skew S. Remarkably, this K-S inequality is found to be satisfied by circulation variables even in the observed multi-component climate system. A principle of Diagonal Dominance in the multi-component moment equations is introduced to understand this behavior.

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**MS28**
**A Complex Systems Modeling and Emulation Approach to Cybersecurity**

There are at least two different ways of approaching complexity: the study of the combinatorially large (Turing's halting problem, decidability, etc.) and the study of self-organization on the edge of criticality (mathematical biology, etc.). Results will be presented that support both of these approaches as tools for understanding the cybersecurity problem. The first puts limits on what can be discovered on arbitrary program/machine combinations, requiring us to resort to heuristics or find ways to make the program/machine simple enough to render it susceptible to analysis. The second, referring to work in Highly Optimized Tolerance, is capable of making non-local, often qualitative predictions about the behavior and topology of highly evolved systems over time. From this, conclusions will be drawn about fundamental differences between the current cyber-security problem and standard problems in security, and why it is both vastly harder to solve and more prolific.

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**MS28**

**Cyber Analytics Challenges and Solutions for Computer Security**

Cyber analytics is the science of data analysis applied to cyber data. Three areas of challenge are (1) observation-gathering and viewing the vast quantity of cyber data, (2) hypothesis generationmaking sense of the data with explanatory stories, and (3) hypothesis testingcomparing accuracy among proposed hypotheses to gain a true understanding. We present these challenges, some solutions, and a research agenda for collaborative efforts between the cyber and applied math communities in cyber analytics.

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**MS28**

**Prediction Methods for Mitigating Computer Security Threats**

Given reliable event predictions, it may be possible to mitigate or even counter computer security threats before they occur. This presentation will discuss the challenges of applying prediction methods to security threats. For example, techniques are needed to quickly find patterns of suspicious activity within volumes of diverse log data. Furthermore, data analysis within a single system and comparison across systems is needed to help determine when things are going wrong and prevent security problems.

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**MS28**

**Applying Formal Methods to a Cross-Domain Component: Lessons Learned and Future Directions**

Galois Inc.'s *Block Access Controller* (BAC) mediates all disk block accesses across security domains, and is a critical security component in our multi-level secure file server. Using the Isabelle proof assistant, we have formally verified that the BAC enforces its safety and data separation policies. This talk will focus on the verification engineering process: why we needed a proof assistant, the verification challenges we encountered, and how we want to make it easier to verify future cross-domain components.

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**MS29**

**A Numerical Method for Thin Flexible Bodies Coupled to Vortex Sheets**

We describe an efficient numerical method for a challenging class of coupled fluid-solid interaction problems. A thin inextensible fiber moves passively or under active driving forces according to a nonlinear beam equation in an inviscid flow. Vortex sheets emanate from the edges of the fiber and roll up according to the Birkhoff-Rott equation. Using an implicit formulation we circumvent numerical instabilities related to the production of circulation. We also implement a gradual smoothing of vorticity near the body edges for improved accuracy. We present results for two physical problems.

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**MS29**

**Fictitious Domain-Like Methods and High Order Finite Elements**

The Fat Boundary Method (FBM) is a fictitious domain-like method for solving partial differential equations in a domain with holes, and more generally fluid/structure problems. One of its interests is the capability to use simple structured meshes (basically Cartesian grids) which do not generally match the boundaries of the holes. This makes it easier the use of fast solvers. The main idea consists in splitting the initial problem into two new ones to be coupled via Schwartz type iterations. A "Global" one, for which the solution is computed using a fictitious domain-like approach in the whole domain (including the holes), and a "Local" one, aims to correct the computed solution in a narrow strips around the holes. In the framework of a finite element discretization, most of fictitious domain-like methods don't preserve the optimal order, especially when high order discretizations are considered. Obviously, this is mainly due to the use of non-boundary fitted meshes. In this work we present some numerical experiments showing the usefulness of this kind of methods. On the other hand, and as opposed to other fictitious domain-like methods, we present a sketch of the proof of an optimal error estimate for the FBM. This property is basically due to the local resolution in the vicinity of each hole. (joint work with Silvia Bertoluzza and Bertrand Maury)

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**MS29**

**Dynamics of 3D Axisymmetric Vesicles**

Abstract not available at time of publication.

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**MS29**

**Dynamics of Suspension of Semi-flexible Filaments**

In this study we investigate the dynamics of semi-flexible

filament suspension using numerical simulations and kinetic theory. The filaments are flexible and interacting with each other in the Stokes fluid, and in the dilute limit we employ the slender-body formulation for each semi-flexible filaments with hydrodynamic interaction and lubrication force when they are in close range with neighboring filaments. We also employ kinetic theory to describe the rheology of flexible filaments and use these results to interpret the simulations.

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**MS30**

**Numerical Analysis of the Navier-Stokes/Darcy Coupling**

We present mathematical and numerical models for simulating incompressible fluid flows through porous media. The main applications of our interest are the hydrological environmental ones and mass transfer in biomechanics. We outline the analysis of a coupled Navier-Stokes/Darcy problem. After proving its well-posedness using the Beavers and Joseph interface conditions, we introduce a stable Galerkin finite element approximation and we study effective iterative schemes based on domain decomposition theory to compute its solution.

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**MS30**

**Operator Splitting Multiscale Finite Volume Element in Multiphase Flow Simulation**

A numerical method for solving two-phase flow problem is investigated in the setting of physics-based two-level operator splitting. The governing equations involve coupled elliptic differential equation with parabolic convection-dominated equation which pose a severe restriction for obtaining numerical solution in fully implicit manner. Strong heterogeneity of the porous medium over many length scales adds to the complicating factors for effectively solving the system. One viable approach is to split the system into three sub-system: the elliptic, the hyperbolic, and the diffusion equation, respectively, allowing the use of numerical discretization appropriate for each one, and exchange of information between them. We propose to use the Multiscale Finite Volume Element (MsFVEM) for elliptic and diffusion equations, and a non-oscillatory difference scheme for the hyperbolic equation, capable of capturing the front in the solution. Performance of this procedure is confirmed through several numerical experiments.

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**MS30**

**Adaptive and Locally Conservative Numerical Methods for Two-Phase Flow in Porous Media**

Two-phase flow in porous media has important applications for petroleum reservoir engineering and groundwater processes. Both applications may involve multiple time and spatial scales, long simulation time periods, and many coupled nonlinear components. In particular, the advection-dominated component and the nonlinear coupling of compressibility, capillary pressure and relative permeabilities often result in sharp saturation fronts, which demands steep gradients to be preserved with minimal oscillation and numerical diffusion. In this talk, we consider the combined method of discontinuous Galerkin (DG) and mixed finite element (MFE) for simulating two-phase flow in porous media. A number of numerical examples are presented to illustrate computational advantages of DG methods for porous media flow, with emphasis on the treatment of capillary pressure heterogeneity and the dynamic mesh modification.

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**MS30**

**A Finite Volume Method for the Stokes Equations**

We develop a finite volume method for solving the Stokes equations. In this method, $BDM_1$ element is used to approximate velocity. As a consequence, this finite volume solutions feature a full satisfaction of divergence free constraint. Optimal-order error estimates are established for the corresponding finite volume solutions in various Sobolev norms. Numerical examples are provided.

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**MS31**

**Memory-aware Scheduling for Parallel Out-of-core Multifrontal Factorizations**

In this talk, we study the memory scalability of the parallel multifrontal method, a particular sparse direct method. We first show that maximizing coarse-grain parallelism and minimizing memory usage are contrary objectives. We then propose an algorithm achieving a high memory scalability but restricted to fine-grain parallelism. Finally, we propose an algorithm that exploits the available memory to maximize coarse-grain parallelism. Experimental results on large matrices illustrate the discussion.

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**MS31**

**Sparse Matrix-matrix Multiplication for Accelerating Parallel Graph Computations**

Parallel computations on petascale graphs require highly scalable algorithms. Those graphs, often arising from fields like computational biology and web analysis, are irregular and unstructured. Computations on graphs would benefit from more coarse-grained parallel primitives, as the computation time is often dominated by latency. We describe the usage and implementation of sparse matrix-matrix multiplication on a general semiring. As a coarse building block, it can be used to accelerate many graph algorithms.

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**MS31**

**A Parallel Half-Approximation Algorithm for the Weighted Matching Problem**

We present a parallel half approximation algorithm for the maximum weight matching problem. The approximation is guaranteed through local weight dominance. The communication cost is proportional to the size of the edge cut of the partitioned graph. Computational results on a distributed-memory machine using hundreds to thousands of processors indicate that the algorithm represents a good candidate for computing approximate weighted matchings on very large graphs.

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**MS31**

**A New Heuristic for Bipartite Matching Algorithms**

It is a well established result that improved pivoting in linear solvers can be archived by computing a bipartite matching between matrix and diagonal entries. With the availability of increasingly faster linear solvers, the speed of bipartite matching computations must keep up to avoid slowing down these solvers. Fast algorithms for bipartite matching which are usually initialized with simple heuristics have been known for a long time. However, the performance of these algorithms is largely dependent on the quality of the heuristic. We present a new heuristic aimed at obtaining high quality matchings and compare its impact on bipartite matching algorithms with that of other heuristics, using real-world matrices as well as randomly generated testcases.

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**MS32**

**Multi-species Lattice Boltzmann Models and Applications to Sustainable Energy Systems**

Multispecies modeling is important in many practical applications relevant to sustainable energy systems, such as chemical/electrochemical reactions, controlled combustion and pollutant dispersion. The Lattice Boltzmann Method (LBM) is considered a promising tool for solving equations, because it allows one to take into account interactions among fluid particles. In this talk, some popular minimal kinetic models are discussed and some results are reported concerning microstructured electrodes for solid oxide fuel cells (SOFC).

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**MS32**

**Applying Lattice Boltzmann Flow Solver for Medical Simulations**

The coupled simulation of blood flow, species transport and biological processes in patient specific vessel geometries play an increasingly important role in medical physics, with the ambitious goal to help clinicians with risk prediction and treatment planning. In this presentation we describe various approaches of applying Lattice Boltzmann flow solvers in environments requiring CFD-simulations in the framework of medical physics, such as blood flow simulation within cerebral aneurysms and a coupled multiphysics multi-scale simulation of flow-induced biological processes.

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**MS32**

**waLBerla: Large Scale LBM Simulation of Moving Particles**

Particulate flows are widespread in nature and industrial applications. In this session we study the methodology behind the simulation of fluid flow with more than 100,000 fully resolved rigid bodies incorporated in the flow. Besides the basic numerical methods behind both the fluid simulation and the rigid body simulation, the necessary extensions and the coupling between both methods are presented. Furthermore, the parallelization of the system is discussed and performance results are given.

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**MS32**

**Simulation of Viscous Flow and Colloid Transport in Saturated Soil Porous Media**

The transport and retention of sub-micron colloids in soil are governed by both physicochemical forces near grain surfaces and hydrodynamic forces due to pore-scale viscous flow. Here we report on a computational model designed to allow a systematic study the colloid transport and retention. Several important issues related to the mechanism and quantification of colloid retention will be discussed in light of the simulation results.

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**MS33**

**Adaptive Immersed Boundary Methods for Simulating Cardiac Fluid Dynamics**

In this talk, I shall describe an adaptive version of the immersed boundary (IB) method and the application of this method to problems of cardiovascular fluid mechanics. Additionally, I shall present results from the three-dimensional simulation of blood flow through a model of a natural aortic valve and a model of a chorded prosthetic mitral valve, as well as to the simulation of whole heart fluid-muscle-valve mechanics.

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**MS33**

**Surface Phase Separation and Flow in Vesicle Bio-membranes**

Abstract not available at time of publication.

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**MS33**

**Accurate Tree-Based Adaptive Volume-Of-Fluid for Surface-Tension-Driven Flows**

I will present recent developments in the quad-octree Gerris Flow Solver (http://gfs.sf.net) which allow adaptive simulations of interfacial flows. In contrast to previously published techniques, Gerris allows for mass-conserving adaptivity along the interface. Extension to the quad-octree of the height-function curvature estimation and "balanced-force" CSF formulation of surface tension leads to highly accurate results for classical surface tension test cases. I will conclude with a selection of applications illustrating the capabilities of the Gerris solver for difficult interfacial flow problems.

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**MS33**

**Simulations of Physical Phenomena Using GERRIS**

Abstract not available at time of publication.

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**MS34**

**Coupling of Biochemistry and Stresses and the Mechanism of Lung Airway**

Abstract not available at time of publication.

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**MS34**

**Kinematic Transport Properties in Energetic Variational Approaches for Complex Fluids**

Abstract not available at time of publication.

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**MS34**
**New Phases in Biaxial Liquid Crystal Polymers**

Abstract not available at time of publication.

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**MS34**
**Kinetic Theories for Complex Fluids Flows**

Abstract not available at time of publication.

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**MS35**
**An Iterative Method for Parameter Estimation in Porous-Media**

The representer method was originally proposed for data assimilation in oceanography. The method solves the Euler-Lagrange equations arising from minimizing the data misfit subject to model constraints, by reducing the problem to the computation of "representer" functions and an expansion of the solution in terms of a forward model solution and the representers. For linear problems, the method is exact. For nonlinear problems such as those arising in parameter estimation, we propose an iterative representer based scheme, whereby the representer method is applied to the Euler-Lagrange equations arising from the minimization of the data misfit subject to the constraints imposed by the first order conditions applied to the nonlinear model. We also describe the combination of the representer method for determining geologically consistent representations of the unknown permeability, described using a Karhunen-Loeve expansion. Theoretical results for single phase flow problems will be described and numerical results for single and two phase flow will be given.

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**MS35**
**Analysis of the Effects of Routing Strategies on Stochastic Networks**

We discuss the modeling and simulation of large stochastic networks in which the propagation of information through the network is governed by probabilistic rules. We are interested in understanding the effects of routing strategies that vary the tendency of transmission depending on the state of the network and of the effects of interference between network nodes. Since direct simulation of a large stochastic network is prohibitively expensive, we use a continuum model for the expected value of the queue in each node to carry out an analysis of the various network models. The continuum model is a nonlinear parabolic problem that is solved with sophisticated numerical methods very rapidly.

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**MS35**
**Computations of Self-organized Cooperative Behaviour in Shallow Water Flows**

Computations of the statistical equilibria of a Shallow Water Model for low energy non-QG flows on Jupiter, predict in a SINGLE most probable state several large-scale features of the Jovian atmosphere, including (I) anticyclonic predominance through an energy gap due to the large planetary spin, (II) high rim velocity in the Great Red Spot and (III) an alternating zones-belts banded structure. Numerical evidence suggests that these features self-organize through a first order phase transition at an intermediate positive value of the temperature or Lagrange multiplier for the energy-momentum reservoir comprising of the small scales and the massive rotating planet.

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**MS35**
**An Efficient Numerical Scheme for the Boltzmann-BGK Model Using a Spectral Sparse Representation**

We shall present a new spectral method for solving high-dimensional PDEs. The method is based on two basic ingredients: (i) Choosing the frequencies of the trial functions from the "hyperbolic cross"; (ii) Using a suitable sparse grid to perform the numerical integration. We shall provide rigorous error estimates for the proposed numerical method and present numerical results to support our theoretical estimates. The new method will be applied to the numerical simulation of the Boltzmann-BGK model.

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**MS36**

**A Computational Study of Extragalactic Jet Stability**

Observations of extragalactic jets show highly collimated structures that extend over distances which are many orders of magnitude larger than the central object from which they emanate. An important question for magnetically dominated jets is how they remain robust to the kink-type instability which is observed in pinched laboratory plasma configurations. Here, we present a study of the stability properties of these systems via nonlinear non-relativistic 3D magnetohydrodynamic (MHD) finite element computations. Using a logarithmic mesh to resolve multiple length scales, these simulations produce collimated outflows that are significantly larger than the shearing scale of the accretion disk. Confirmed by an eigenmode analysis, the results show that the Coriolis effect in the rotating jet stabilizes the kink mode.

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**MS36**

**Divide and Conquer - Quantum Style!**

Systems are often simulated using a 'divide and conquer' strategy which splits them up into a vector of independent elements and a matrix of couplings. However, this makes the assumption that the system can be meaningfully described (at fixed time) by describing each part. In the world of quantum mechanics, this assumption no longer holds. In this talk, I shall describe how this happens, and introduce 'tensor network algorithms' which accommodate this situation.

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**MS36**

**Virtual Photons in Imaginary Time: Computing Casimir Forces Using Standard Numerical Electromagnetism Techniques**

The quantum vacuum is teeming with virtual photons that give rise to forces between neutral macroscopic objects. In particular, the zero-point energy of the electromagnetic field can give rise to attractive (and in special circumstances, repulsive) forces between neutral objects. Casimir forces depend strongly on the shape and material properties of these bodies, but calculations are difficult and have been restricted to two-dimensional perfect-metal geometries or to additive pairwise approximations that have been shown to yield quantitatively incorrect results. We developed a new computational method with which it is possible to calculate exact Casimir forces in arbitrary geometries and materials (an exemplary case of a simulation-based scientific approach to the engineering of these microstructures). Using this method, which frames the problem of computing the forces in terms of standard numerical electromagnetism techniques, we investigate a number of unusual effects, including the first instance of a non-monotonic force in a many-body geometry and the levitation of microscopic objects via repulsive Casimir forces. The latter study is the first demonstration of stable equilibria between realistic objects of finite extent and is therefore a significant step in the study of possible passive-suspension devices at the nano-scale

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**MS36**

**Probing and Utilizing Coarse Variables Using Diffusion Maps**

Many high-dimensional problems in science and engineering have spatial or temporal dynamics of a much smaller dimension. Using ideas from machine learning, we probe for this low dimensional representation by looking at the spectrum of diffusion operators on the data sets generated by these scientific problems. The resulting low-dimensional description allows us to do things like projective coarse integration, free energy calculations, bifurcation analysis, etc.

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**MS37**

**Osteoporosis: A Mathematical Perspective**

Osteoporosis is a common age related chronic disorder of the skeleton. It constitutes a considerable public health problem, with the number of Americans affected estimated at about 15 million. I will present an overview of osteoporosis, give a quick tour of the bone remodeling process, and describe the fundamental elements involve in determining bone strength in vivo. The talk will show why mathematics is playing an increasingly relevant role in the research, diagnosis, and monitoring of osteoporosis.

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**MS37**

**Rate Allocation in Reservoir Management**

Constrained optimization problems arise naturally in many activities related to the production of oil and gas. The derivatives or sensitivities computation of both the optimization models objective function and the constraints is a critical ingredient in derivative-based optimization algo-

rithms. This talk will focus on one problem related to injection rate allocation in reservoir management.

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**MS37**

**Better Preprocessing for Industrial CFD: More Important Than You Might Think**

Computational analysis preprocessing for complex industrial models can be very time-consuming and require much engineering expertise. Model preprocessing, which includes geometry-model preparation and mesh creation, consumes up to 75% of total analysis cycle time in practice. For computational fluid dynamics (CFD) analyses at Boeing, I will present examples of model-prep issues impacting design-cycle throughput. I will also discuss techniques to mitigate these problems through better automation of geometry prep and mesh generation.

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**MS38**

**Interdisciplinary Mentoring Program in Analysis, Computation, and Theory**

Each year, BYUs math department runs an undergraduate research training program. This begins each summer term with a 7-week intensive boot camp experience that prepares students (primarily math majors) to begin their individual research projects in the fall. Students develop the mathematical, statistical, and computational foundation needed to do interdisciplinary research through highly-integrated assignments and computer labs. After the summer, the students break off and work on their own research projects.

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**MS38**

**The Computational Mathematical Sciences Program at Arizona State University**

I will describe aninnovative baccalaureate program that has a significant component in the computer, physical and/or life sciences in addition to the usual core mathematics courses. Qualified students may participate in intensive, NSF-funded, 8-week summer research experiences in atmospheric science, cancer dynamics, scientific visualization, fluid dynamics, and financial mathematics. Challenges, opportunities, and suggestions for faculty trying to develop similar programs will be discussed.

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**MS38**

**Mathematical Sciences and Computation at NJIT: Undergraduate Research and Curriculum**

Research in applied and computational mathematics plays an important role in the Department of Mathematical Sciences at the New Jersey Institute of Technology. Efforts to integrate mathematical sciences and computation have always been a focal point of the undergraduate curriculum offered by the department. This has been formally facilitated in the past two years through the NSF funded CSUMS program. Cohorts of 6-8 undergraduate mathematical science students are exposed to scientific computing through an extension of the curriculum in parallel to immersion in rigorous research programs. These introduce participants to state of the art computational techniques and methodologies. Research projects within the NJIT CSUMS program canvas many different areas within the mathematical sciences, employing deterministic and stochastic techniques to study problems in areas such as fluid mechanics, wave propagation, and inverse problems. An important component of our program is the group nature of the proposed activities, including team projects supervised by multiple faculty mentors, frequent group meetings, workshops in scientific computation, and social activities. With a significant group of students at our institution interested in pursuing mathematics of finance and actuarial science, we have also extended our curriculum to include senior level computational financial mathematics classes. Further complementing CSUMS efforts, a B.S. degree in Computational Science has been recently established with new courses on employing scientific computing to tackle problems in applied science (mathematics, biology physics, chemistry).

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**MS38**

**Computational Science: Coursework and Mentoring**

Two tracks for undergraduate computational mathematicians at George Mason University are described. Following project-oriented numerical mathematics courses, students have a choice of pursuing computational mathematics or computational science majors. Upper-level undergraduates may enter the NSF-supported CSUMS program, a year-long participation in mentored research on computational science.

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**MS39**

**Overcoming Challenges in the Scalability of Uintah**

The Uintah code is a complex fluid-structure interaction code that has been developed over a dozen years at the

University of Utah with DOE funding. Novel features of the code include fully automated parallelism and a very broad problem class. Recent results based on new algorithms and analysis of the code have greatly improved scalability of the code. Algorithms, analysis and results from runs on many thousands of processors using adaptive mesh refinement will be shown.

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**MS39**

**Scalable Adaptive Mantle Convection Simulation on Petascale Supercomputers**

We present a library for dynamic mesh adaption and redistribution that is designed for petascale systems. The library uses parallel octree-based hexahedral finite elements and dynamic load balancing based on space filling curves. We use the library to conduct high resolution mantle convection simulations that resolve thermal boundary layers and faulted plate boundaries, down to 1 km scales. We present scalability and performance data on up to 62K cores of Ranger, the 580 Teraflops system at TACC.

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**MS39**

**Performance Analysis of an Adaptive Computational Fluid Dynamics Solver on Near Petascale Supercomputer Systems**

PHASTA is a parallel implicit finite-element based CFD code. This presentation will discuss the scaling of PHASTA's core algorithms across a number of current near petascale systems, including Blue Gene/L, Blue Gene/P, Cray XT3, and Sun Constellation Linux Cluster. Specific attention will be paid to maintaining strong scaling on large numbers of cores, and procedures to manage adaptive meshes where the number of elements may change by orders of magnitude during the simulation.

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**MS39**

**Advancing Energy through Algorithms Despite Architectures**

In developing both plasma fusion and next generation fission concepts, simulations are expected to guide expensive experimental programs. We review the algorithmic agendas of recent reports of the U.S. Department of Energy for these novel energy technologies, and illustrate with prototype and at-scale distributed computations. We point out where today's algorithms of choice are likely to be shoaled by memory or memory bandwidth limitations of emerging architectures.

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**MS40**

**Petascale Computing for Storm Surge and Hydrodynamics**

Abstract not available at time of publication.

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**MS40**

**A Discontinuous Galerkin Storm Surge Model**

In this talk we report on progress toward the development and application of a next generation hurricane storm surge model that uses a discontinuous Galerkin (DG) method for the solution of the governing shallow water equations (SWE). DG methods are a family of finite element methods particularly well suited for this type of problem. The DG model incorporates a robust, mass conservative wetting and drying algorithm and a parallelization strategy that displays excellent scalability.

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**MS40**

**Computational Speedup Results for Storm Surge Simulations Using FPGAs**

Certain numerical algorithms can be implemented on field programmable gate arrays (FPGAs) to achieve speedup. In this talk, I will present speedup results obtained on FPGA simulations of a numerical code that implements the discontinuous Galerkin method for solving PDEs that model storm surges. The work indicates that hybrid computer systems might be a promising direction for obtaining desirable numerical speedup results.

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**MS40**

**Verification and Validation of High Resolution Hurrice Wind, Wave and Surge Simulators**

Abstract not available at time of publication.

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**MS41**

**Analyzing Emergent Behaviour in Cellular Automaton Models of Cancer Growth**

Deciphering the principles of tumour growth is crucial for the development of new therapy concepts. Besides increasingly complex molecular investigations, mathematical modelling and computer simulation of selected aspects of tumour growth have become attractive within the last few years. Here, we focus on the analysis of cancer invasion. Lattice-gas cellular automaton models allow for an adequate description of individual invasive cancer cell behaviour (microscopic level). We will show how analysis of the models allows for prediction of emerging macroscopic properties (in particular of the invasion speed). Furthermore, we will show how to apply our models to the interpretation of data from in vitro glioma cell assays.

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**MS41**

**An In-silico Model of the Role of Apoptosis and Migration in Three-dimensional Tumor Growth**

Cancer development may be considered an evolutionary process whereby genetically unstable cell clones compete under selective influences of the local environment and succeed in accordance with the relative fitnesses of their expressed phenotypes. We show theoretically how tumor populations devoid of stem cells could still persist as long-term dormant lesions, and offer a possible explanation for the incidence of dormant tumors observed in recent autopsy studies. This finding questions the notion that tumors escaping dormancy will necessarily become symptomatic. Finally, if the tumor population is assumed to contain cancer stem cells, we show 1) that certain conditions may paradoxically limit the growth of the lesion, even if it escapes dormancy, and 2) the number of stem cells can be amplified through adjustments in other parameters that reduce the local density of progeny cells. The latter observation lends support to the theory that tumors grow in part through the creation and merging of local metastases. From the presented model we derive implications for treatment.

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**MS41**

**Modeling of Avascular and Vascular Tumors Using the GGH Model and CompuCell3D**

While numerous computational tools are available for analysis of DNA sequences, network reaction kinetics and molecular dynamics, multi-cell modeling of developmental processes is less sophisticated. Now, a growing community of modelers use the GGH Model to create multi-cell simulations of tissue development. I will present GGH simulations of the front instabilities of a simple model of growing avascular tumor spheroids and more sophisticated models of tumor vascularization, implemented in the open-source modeling environment CompuCell3D (www.compucell3d.org).

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**MS41**

**Growing, Breaking, Migrate and Invade – What Can We Learn from Mathematical Models of Can-**

**cer**

In this talk a brief overview of distinct aspects of tumor development and its progression will be given and different modeling techniques highlighted to set up a background for the minisymposium. I will then concentrate on the initiation and early development of ductal breast tumors and will present the results of computer simulations of the IBCell model showing the formation of normal and tumor-like epithelial ducts and distinct forms of ductal carcinomas in situ.

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**MS42**

**Modeling the Impact of an Epidemic on Network Topology**

In models of epidemics on contact networks, the probability of exposure is determined by the connectivity (degree) of the individual (node). We find that the structural evolution of the network varies with its topology and the contagiousness of the disease. We identify mechanisms to make them sparser and study questions about the patterns of immunity that arise during disease outbreaks and the impact of past epidemics on the dynamics of future outbreaks.

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**MS42**

**Modeling Communicable Disease Spread: New Tools for an Old Problem**

The underlying contact structure among individuals that determines the pattern of disease transmission and the progression of this pattern over time are two crucial elements in understanding and controlling communicable disease spread within a social setting. Recent advances in mathematical modeling have provided us the means to tackle emerging infectious disease concerns head-on; these new tools can play a crucial role in public health decision-making at times of crisis. This talk aims to describe the concepts and applications of these new techniques in communicable disease control. We demonstrate how these tools can be used to address pandemic influenza preparedness as well as preparedness plans for the natural or deliberate release of infectious agents during a major public event.

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**MS42**

**On Realizing All Simple Graphs with a Prescribed Degree Sequence**

We give a necessary and sufficient condition for a sequence of nonnegative integers to be realized as a simple graphs degree sequence such that a given (but otherwise arbitrary) set of possible connections from a node are avoided. We then use this result to present two algorithms, one that builds all simple graphs realizing a given degree sequence and another one which samples uniformly at random from this set of graphs.

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**MS42**

**The Structure of Social Contact Networks and their Impact on Epidemics**

We will explore some of the important structural properties of large-scale realistic social contact graphs, which have a significant impact on disease dynamics. One such measure is node vulnerability, which is the probability that a node gets infected, starting at a random initial infection. We show that vulnerability is very different from other graph measures, and leads to much better strategies for reducing the spread of epidemics.

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**MS43**

**Compressive Wave Computation**

This talk presents a strategy for computational wave propagation that consists in decomposing the solution wavefield onto a largely incomplete set of eigenfunctions of the weighted Laplacian, with eigenvalues chosen randomly. The recovery method is the ell-1 minimization of compressed sensing. For the mathematician, we establish three possibly new estimates for the wave equation that guarantee accuracy of the numerical method in one spatial dimension. For the engineer, the compressive strategy offers a unique combination of parallelism and memory savings that should be of particular relevance to applications in reflection seismology

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**MS43**

**Complete Plane Wave Representations and Optimal Radiation Boundary Conditions**

We develop a novel representation of solutions of the wave equation in a half-space and use it to construct local radiation boundary conditions. We prove that with $O\left(\ln\frac{1}{\epsilon}\cdot\ln\frac{cT}{\delta}\right)$ auxiliary functions we achieve a relative accuracy of $\epsilon$ up to time $T$ if all sources and scatterers are separated by at least $\delta$ from the artificial boundary. Numerical experiments are presented which verify the accuracy and efficiency of the new method.

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**MS43**

**Calderon Preconditioned Time Domain Integral Equation Solvers for Electromagnetics**

Please enter your abstract here. Seventy-five (75) word

maximum. Do not include self defined TeX commands. Marching on in time integral equation solvers for analyzing broadband electromagnetic phenomena often suffer from spatial (dense-mesh) breakdown phenomena when applied to the analysis of low- to medium-frequency electromagnetic transients on geometrically intricate and multiscale structures. This presentation highlights the recent development of Calderon-inspired quasi-analytical preconditioners that address this breakdown phenomenon and demonstrates its application to engineering problems that span multiple temporal and spatial scales.

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**MS43**

**Accelerating the DG Time-Domain Method**

We will discuss the performance of graphics processing unit (GPU) accelerated implementations of the discontinuous Galerkin (DG) method for time-dependent electromagnetics computations. Modern GPUs consist of hundreds of compute units that are able to support up to thousands of lightweight, concurrent threads. We will discuss how the DG method can be mapped efficiently unto example GPU cards from nvidia and AMD. Computational examples will be presented to demonstrate the level of performance attainable on these platforms.

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**MS44**

**Coupled Atomistic-continuum Methods for Fluids**

Abstract not available at time of publication.

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**MS44**

**A New Spectral Moving-mesh Method for the Phase-field Model for**

Abstract not available at time of publication.

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**MS44**

**Defect Detection and Tracking Algorithms in 2-d and 3-d Hydrodynamics of Nematic Liquids**

Abstract not available at time of publication.

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**MS44**

**Highly Entangled Wormlike Micellar Solutions: Model and Predictions in Shearing Flows**

Wormlike micelles and monodisperse polymer mixtures are both entangled solutions thus have viscoelastic properties. Experimental studies have shown that steady and transient shearing flows of these solutions exhibit spatial inhomogeneities in flow, such as 'shear-banding', at sufficiently large applied shear rates. In the present work, we investigate the dynamical response of a class of two-species models which can capture, in a self-consistent manner, the creation and destruction of an elastically-active network segment, as well as diffusive coupling between the microstructural conformations and the local state of stress. For each of these models, the steady state calculations of the full inhomogeneous flow field lead to localized shear bands that grow linearly in extent across the gap as the apparent shear rate is incremented, and a plateau in the shear stress shear rate 'flow curve'. Large amplitude oscillatory shear (LAOS) deformations are used to systematically explore the complex dynamics of shear-banding over a wide rage of strains and frequencies. A 'phase diagram' capturing the different type of banding events, as well as the special limiting cases of linear viscoelasticity and of steady inhomogeneous shear flow, is developed using a Pipkin space representation. Portions of this work were done with support of NSF-DMS under DMS#0405931 and DMS#0406590

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**MS45**

**Link Prediction on Evolving Data using Tensor Factorizations**

There are many social networks that have massive amounts of data evolving in time. The analysis of such datasets requires methods capable of modeling large, multi-modal and sparse datasets. We rearrange time-evolving data as a third-order tensor and find the underlying factors in different modes based on tensor factorizations using optimization. We use the extracted factors to build predictive models and assess the performance of our approach in the context of link prediction on a bibliographic dataset.

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**MS45**

**Tensor-based Regression**

In omics (bioinformatics, metabonomics etc.) complicated data structures often arise. In this presentation, several such data will be presented and it will be shown how linear regression can be extended to multi-way tensor regression.

Tensor regression produces much more parsimonious regression models than alternative matrix-based models and lead to more robust predictions as well as easier interpretation of the models. The importance of these aspects will be highlighted.

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**MS45**

**Kernel-based Extension of Tensor Decomposition for Face Recognition**

Tensor decomposition has been successfully applied to dimensionality reduction of face images changed by multiple factors such as different people, poses, or illuminations. In this talk, we introduce Multilinear Kernel Principal Component Analysis (MKPCA), a combination of tensor decomposition with a well-known nonlinear subspace method, Kernel Principal Component Analysis. The subspaces obtained using MKPCA are nonlinear as well as multilinear, which makes MKPCA applicable to real-world data that often have nonlinear distribution and multiple factors.

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**MS45**

**Incremental Tensor Decompositions for High-order Data Streams**

In this talk, we introduce a general framework Incremental Tensor Analysis (ITA) which efficiently computes a compact summary for high-order and high-dimensional data, and also reveals the hidden correlations. Three variants of ITA are presented: 1) dynamic tensor analysis (DTA), 2) streaming tensor analysis (STA) and 3) window-based tensor analysis (WTA). In particular, we explore several design trade-offs. Finally, we present some interesting patterns and outliers on the real datasets.

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**MS46**

**Simulation of Particulate Air Filtration in Media Formed from Capillary Channel Polymer Fibers**

We simulate high efficiency particulate air (HEPA) filtration, comparing a filter consisting of capillary-channel polymeric (C-CP) fibers with a round-fiber filter. C-CP fibers have longitudinal grooves which significantly increase their surface area in comparison to round fibers, resulting in interesting properties for filtration and separations applications. Numerical techniques including domain set-up, grid generation, finite element solution, and Brownian dynamics simulation will be discussed. Pressure drop and filter efficiency results under various conditions will be presented.

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**MS46**

**Coupled Groundwater Flow and Heat Transport for Large-Scale Remote Sensing Studies**

In an effort to improve synthetic thermal imagery for remote sensing technologies, a suite of closely coupled numerical simulators has been developed. This computational testbed includes thermal and moisture transport finite element models, coupled with solar and vegetation models. It is well suited for simulations of specific scenarios, which otherwise might be difficult and time consuming to reproduce in the field. This talk will focus on the code coupling and challenges encountered with large-scale simulations.

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**MS46**

**Optimization As a Tool for Understanding Polymer Filter Designs and Layer Configurations**

We pair a 3-D simulator that models non-Newtonian flow of a polymer through a filter with derivative-free optimization techniques to determine optimal filter parameters. We provide numerical results for three different measures of filter performance which use a barrier term to account for escaped debris and compare the performance of the filter using a one layer versus two layer configuration with optimal parameters.

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**MS46**

**Modeling of Debris Deposition in an Extrusion Filter Medium**

In this talk, we discuss a simulation tool for modeling debris deposition in a filter medium. The application arises from an industrial fiber-spinning process, where an extrusion filter separates debris particles from the polymer melt before it is spun into the finished product. We use mass balance and particle transport equations adjusted for non-Newtonian fluids. We also include equations that model debris capture. We provide numerical results and discuss directions for future research.

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**MS47**

**Earthquake Simulation: From Rupture to Virtual City Response**

The major goal of this work is to implement physics-based analyses that correctly model the complete earthquake process, from source rupture to the response of the entire built environment in the affected region, including the interaction between separate structures through the soil. We illustrate the capabilities with a large scenario earthquake in southern California, and describe how we use the ground motion over an entire earthquake-prone region toward the simulation of urban earthquake impacts.

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**MS47**

**A General Abstraction to Support Adaptive Multiscale Multiphysics Simulations**

Current simulation software does not interact with a general abstraction of the problem to be solved. This is a key reason that even though adaptive procedures have been extensively studied, they are still not widely used. An abstraction of multiscale multiphysics simulations that supports adaptive control of models and discretizations will be presented. The abstraction is being implemented as a set of components and applied to multiple applications including biotissue design and concurrent multiscale applications.

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**MS47**

**Parallel Computing for Accelerator Design and Modeling**

Electromagnetic simulation of large and complex accelerator systems using the finite-element approach with unstructured grids on state-of-the-art supercomputers requires advanced scalable computational techniques and numerical algorithms. Advances in some of those techniques such as scalable linear and eigen-solvers, parallel adaptive refinement, and dynamic load balancing in the large-scale accelerator simulation will be presented. Additional computational challenges including scalability of memory-usage and parallel I/O will be discussed.

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**MS48**

**Challenges in Multiphysics Mesh Adaptation, Error Indicators, and Data Transfer**

The purpose of this minisymposium is to further the discussion of meshing issues that impact complex multiphysics simulation applications, and possible methods of mitigating these problems. Multiphysics meshing, adaptation, and data management is more demanding than "single-physics" applications due to the need to incorporate requirements from many, possibly tightly-coupled phenomena into the meshing algorithms. This presentation highlights the research topics that are critical to the development of a reliable, timely, and automated multiphysics analysis capability. In particular, the need for and potential impact of solution-based adaptation will be introduced, along with methods of implementing adaptation schemes. Issues involved with the generation of initial mesh(es) and transferring data between meshes in a conservative manner will also be examined.

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**MS48**

**Unstructured Least-Squares Approximation of Rough Data with Surface Spherical Harmonics Ba-**

**sis Functions**

Multi-meshing interpolation and adaptation are becoming quite popular for spatial error control in the numerical simulation of complex computational physics applications. We present an h-p-adaptive least-squares Cartesian method with spherical harmonics basis functions for the approximation of data for solving problems on the sphere, such as climate modeling. The premise of the method is given one or more data fields on the sphere, find a differentiable approximation of the field for the computation of the surface gradient on smooth interpolated data. The proposed method is designed to accommodate unstructured polygonal mesh topologies with a primary goal of resolving local length scales of interest. The interpolation method accepts smooth or irregular data such as earths orography elevation field (satellite) data profile as initial condition (atmosphere depth field and velocity) for the shallow-atmosphere equations.

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**MS48**

**Mesh Generation Tools and Algorithms for Multiphysics Applications**

Abstract not available at time of publication.

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**MS48**

**Remapping - Conservative Interpolation**

We present review of remapping methods for Arbitrary Lagrangian-Eulerian (ALE) methods. We first consider different approaches for remapping of cell-centered quantities. It includes methods based on exact intersection (overlays), swept region integration, flux-corrected remapping and so on. Then we describe remapping of nodal quantities. Finally, we present remapping for multimaterial case.

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**MS49**

**CFD Needs for Nuclear Reactor Simulation**

Today, computational fluid dynamics (CFD) is being used extensively in the nuclear power industry. CFD applications in the nuclear power industry support safe, efficient, and reliable reactor plant operations. As the industry prepares for the development of advanced Generation III and Generation IV reactor designs, the use of CFD will increase dramatically. This presentation highlights specific CFD needs posed by future reactor designs. Topics that will be addressed include the use of CFD as an evalution tool for design certification and licensing, as a design tool for reactor components and processes and as a predictive tool for ensuring safety of future reactor designs. In addition, this presentation includes requirements for verification and validation and uncertainty quantification to support the use of CFD in the design and development of future reactor concepts.

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**MS49**

**Trapezoidal/BDF-2 Time Differencing Applied to Non-Linear Radiation Diffusion and Radiation-Hydrodynamics**

Abstract not available at time of publication.

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**MS49**

**Multiphysics, Multiscale Methods for Nuclear Fuel Performance**

This presentation examines various mathematical and computational issues that impact the thermomechanical response of reactor fuel, and are thus important to the development of INL's fuel performance analysis code, BISON. The code employs advanced methods for solving coupled partial differential equation systems that describe multidimensional fuel thermomechanics. BISON is designed for fully coupled, steady and transient analysis, and is designed to be efficient on both desktop computers and in massively parallel environments. It employs physics-based preconditioned Jacobian-free Newton-Krylov solution methods and is developed using modern software engineering principles to form a robust, extensible software architecture. This discussion summarizes the current status of BISON and demonstrates results on selected 3D fuel performance calculations.

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**MS49**

**Multiphysics LWR Systems Simulators**

Transient systems level simulators for light water reactors involve multiphysics simulation of reactor kinetics, single or two-phase flow and heat transfer, fuel models, models for control, and models for components such as pumps. Here we review our methods for, and our experiences with these system simulators. We also discuss desired improvements.

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**MS50**

**The Multirate Simulation of Power Systems with**

**Power-electronics-based Controllers**

The multirate method is well suited for the numerical simulation of power systems that contain power electronic-based controllers. The presence of power electronic-based controllers leads to system models that contain widely varying time-scale responses due to the sustained high-frequency switching of the power electronics. When there are sustained mid- to high-frequency dynamics in the system, conventional time domain simulation methods are inefficient. However, the computational potential of multirate methods can only be realized if the partitioning between the subsystems accurately reflects the time-scale separations. Partitioning strategies may be difficult to implement in systems that contain both differential and algebraic equations (DAEs). This paper will discuss different strategies for partitioning power electronic-based systems and their impact on computational efficiency and accuracy.

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**MS50**

**Multirate and Co-Simulation Strategies in Chip Design**

In chip design, refined network models yield systems of differential-algebraic and partial differential equations which are coupled via boundary conditions and source terms. These systems can be solved numerically by using the monolothic or dynamic iteration or Co-simulation approach. Whereas multirating is a natural tool in the latter case, the monolithic approach asks for more sophisticated multirate strategies. This talk will discuss both approaches for different examples of refined network models.

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**MS50**

**Multirate Time Stepping for DAEs: Application to Power System Modeling**

For large systems of differential algebraic equations (DAEs), some components may show a more active behavior than others. To solve such problems multirate time stepping schemes can be efficient. With such schemes different solution components can be integrated with different time steps. We show how multirate approach can be applied to power system modeling. The efficiency of the multirate methods is illustrated by the test problems.

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**MS50**

**Compound-fast Multirate Time Integration for IC Simulation**

Circuit models are systems of differential-algebraic equations built by hierarchically organized subcircuits. In our extension of BDF schemes a compound step between course synchronization time points is followed by re-integration of fastly time-varying parts on finer time grids. Dynamic partitioning is according to the local dynamics and complexity of subcircuits. New stability results have been derived for the multirate method. We describe several approaches to treat the interfaces. Results will be demonstrated for problems from circuit simulation.

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**MS52**

**Computational and Modeling Considerations for Structured Multiscale Models of Tumor Invasion**

We will discuss some modeling and computational issues involved in using age structure to represent certain cell level processes in continuous spatial models of tumors, with applicability to other multicellular systems.

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**MS52**

**Computing Cancer Evolutionary Dynamics with Spatial Game Theory**

Evolutionary game theory (EGT), especially after the seminal work of Maynard Smith, has been very successful as a mathematical tool to study the evolutionary dynamics in biological populations. Recent attempts to use EGT to study cancer evolutionary dynamics have been held back by the fact that EGT makes it difficult to account for spatial and environmental influences. In this talk, these limitations and potential computational solutions for a spatial approach to GT will be discussed.

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**MS52**

**A Clinical-scale Model for Glioma Growth and Invasion: Development, Parametrization and Validation**

Computational and mathematical modeling has a novel role to play in the clinical management of cancer patients. Specific examples from the study of primary brain cancer, known as glioma, will be provided to illustrate potential avenues of successful application of patient-specific modeling to not only elucidate biomedical understanding but also suggest novel therapeutic approaches.

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**MS52**
**Multiscale Tumor Modeling**

Based on the concept that tumors behave as complex dynamic and self-organizing biosystems, the talk will describe the development and ongoing refinement of a data-driven, agent-based multi-scale and multi-resolution cancer modeling platform. This algorithm is designed to investigate how changes on the molecular level can percolate across the scales of interest, by impacting microscopic behavior as well as multi-cellular patterns. Applications include simulations of brain cancer as well as lung cancer. This project is part of The Center for the Development of a Virtual Tumor, CViT (https://www.cvit.org), an NCI-supported Integrative Cancer Biology Program.

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**MS53**
**Parallel Preconditioned Harmonic Balance for Analog Circuit Analysis**

Krylov subspace methods with a block-diagonal preconditioner have enabled the steady-state analysis of large analog circuits. However, not all harmonic balance (HB) problems can be solved reliably using the approach. A parallel hierarchical HB method is presented wherein robust preconditioning is provided via the solution of a set of linearized sub-HB problems of decreasing size. These subproblems are constructed implicitly to retain the memory efficiency of Krylov subspace methods.

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**MS53**
**Efficient Transient Noise Analysis in Circuit Simulation**

Noise in electronic components is a random phenomenon that can adversely affect the desired operation of a circuit. Transient noise analysis is designed to consider noise effects in circuit simulation. Taking noise into account by means of Gaussian white noise currents, mathematical modelling leads to stochastic differential algebraic equations. For simulation, we present mean-square convergent adaptive methods together with a new step-size and path control. Numerical experiments on industrial relevant real-life applications illustrate their performance.

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**MS53**
**Linear Solver Strategies for Parallel Circuit Simulation**

While direct linear solvers have long been regarded as a requirement for successful circuit simulation, the parallel transistor-level simulation of large-scale integrated circuits necessitates the use of iterative linear solvers. However, the linear systems generated through circuit simulation are challenging for conventional matrix ordering, load balancing, and preconditioning techniques. We will discuss ongoing work in parallel partitioning and preconditioning techniques that have proven useful for the parallel simulation of large-scale circuits using Xyce.

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**MS53**
**A Non-homogeneous Arnoldi Method for Model Order Reduction of Linear Circuits with Large Number of Terminals**

Large scale RCL circuits with large number of terminals have been widely employed to model interconnect circuits, such as the power/ground networks, clock distribution networks and large data buses in VLSI. In this talk, a Non-Homogeneous ARnoldi (NHAR) process, which consists of a memory-saving and computation efficient linearization scheme and a numerical stable partial orthogonalization Arnoldi method, is proposed for the generation of an orthonormal projection matrix. By applying the obtained projection matrix to generate the reduced-order model, we derive the NHAR(Non-homogeneous Arnoldi Method)for the model order reduction of large scale RCL circuits with large number of terminals. The proposed NHAR method can guarantee moment matching, numerical stability and passivity preserving. Compared with the EXPLIN method, NHAR can remarkably reduce the size of the linearized system and therefore can greatly save the memory consumption and computational cost with almost the same accuracy. Moreover, NHAR is numerically stable and can achieve higher accuracy with approximately the same computational cost compared with the EKS and IEKS methods.

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**MS54**

**Composite Grid Methods for Computational Electromagnetics**

We discuss the solution of Maxwell's equations for complex geometries using composite overlapping grids and high-order accurate methods. The approach is based on efficient methods for Cartesian grids coupled to high-order accurate symmetric finite-volume approximations for curvilinear boundary fitted grids. We use high-order accurate centered boundary conditions and high-order accurate centered approximations at material interfaces. We show the application of the method to solving some deep cavity interface problems.

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**MS54**

**IMEX Methods for Simulating Binary Blackholes**

Inspiral of binary blackholes involves disparate timescales, a long one for orbital motion and a short one on which the gravitational field can potentially change. Overly many explicit time steps are therefore needed to model gravitational wave emission from binary inspiral. We discuss implicit-explicit methods to overcome the CFL restriction in binary evolutions. Our numerical implementation uses the Spectral Einstein Code, a large C++ project developed at Cornell and Caltech by L. Kidder, H. Pfeiffer, and M. Scheel.

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**MS54**

**Generalized Wiener Rational Functions for Spectral Expansions on an Infinite Interval**

The original Wiener rational function basis is a sequence of rational functions orthogonal over the real line, and each basis function decays like $1/x$. We present a generalization of these functions: a basis set that decays like $x^{-n}$ for any $n > 1/2$ over the real line. We demonstrate spectral convergence rates, quadrature, fast computation with the FFT, and an application to a one-dimensional wave problem on an unbounded domain.

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**MS54**

**Boundary Perturbation Methods for High-Frequency Acoustic Scattering: Shallow Periodic Gratings**

Despite significant recent advances in numerical methodologies for simulating rough-surface acoustic scattering, their applicability has been constrained by the limitations of state-of-the-art computational resources. This has been particularly true in high-frequency applications where the sheer size of the full-wave simulations render them impractical, and engineering processes must therefore rely on asymptotic models (e.g., Kirchhoff approximation). However, the demands for high precision can make the latter inappropriate, thus efficient, error-controllable methodologies must be devised. In this talk we present a computational strategy that combines the virtues of rigorous solvers (error control) with those of high-frequency asymptotic models (frequency independent computational costsΘ). These methods are based on high-order boundary perturbations, which display high precision and unparalleled efficiency. This is accomplished by incorporating asymptotic phase information to effect a significant decrease in computational effort, simultaneously retaining the full-wave nature of the approach. The developments of this contribution are constrained to configurations that preclude multiple scattering. Even for single-scattering configurations, the approach presented here gives significant gains in accuracy when compared to asymptotic theories, e.g., KA, with modest additional computational cost.

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**MS55**

**Multicomponent Sorption Modeling in ECBM Displacement Calculations**

Abstract not available at time of publication.

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**MS55**

**A Mixing Model for Aqueous Solutions**

In this paper, we present a mixing model for brine and CO2. The model is an exten- sion of the previously tested theory for H2O + NaCl mixtures which was implemented in a two-phase flow simulator. The incorporation of this model into the mass conserva- tion equations leads to a formulation very similar to the Buckley-Leverett theory, and applies to highly concentrated solutions. In addition, as the governing PDEs for flow and transport are almost de-coupled, a highly efficient numerical algorithm can be applied. When solid salt dissolves in water, the mixture undergoes significant nonlinear vol- umetric effects. Experimental observations indicate that the delta volume of mixing increases with salt concentration, up to a 3% relative change in total volume. However, the volume change is much smaller when water is mixed with saturated brine. Hence, the main assumption of our model is that the delta volume of mixing between two brine solutions at different concentrations (e.g., pure water and saturated brine) is zero. In the scope of geological CO2 sequestration, we are interested in studying the behav- ior of dissolved carbon dioxide in the aqueous phase. Our mixing model can be naturally extended to the ternary systems consisting of water, NaCl and CO2, or by adding an- other chloride salt (H2O, CaCl2 and NaCl). The higher the ionization

of the solutes, the more the important are the nonlinear effects that occur when the salt is dissolved in water, and the assumption becomes less accurate. We show that the model's performance remains unchanged with its extension to ternary systems: the accuracy is not lowered when a second solute of lower ionization is added. The extended model computes den- sity with a maximum relative deviation of Å0.4% and Å1.2% for H2O-NaCl -CO2 and H2O-CaCl2-NaCl respectively, the same deviations as for the binary H2O-NaCl (resp. H2O-CaCl2). Optimizations from the original approach are presented and can halve these maximum deviations. The extension of the model offers a good compromise be- tween accuracy and computational cost, while providing a simple and flexible framework for further extensions.

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**MS55**

**Modeling Density-Driven Fingering In Porous Media: Theory And Simulations**

We will present an application of the recently developed Nonmodal Stability Theory combined with pseudo-spectral simulations to obtain rigorous estimates of the length and timescales for density-driven fingering in porous media. These results will be compared with the critical-times computed by previous investigators. The role played by medium anisotropy will be discussed. We will also present results obtained using layered porous media and discuss the effects of variance and correlation length of the permeability field.

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**MS55**

**Gravity Current of Saturated Brine in Long Aquifers**

Brine saturated with super critical CO2 in deep saline aquifers of large lateral extent spreads as a gravity current along the aquifer floor. The overall dissolution and trapping of CO2 is related to the average density of the current and the rate at which it spreads. These characteristics depend on solubility thermodynamics, density difference, aquifer permeability and orientation. Although the solubility of super critical CO2 in brine is low the current can be driven to large distances leading to substantial dissolution and trapping of CO2. In order to determine the transport characteristics we carry out high-order 3D numerical simulation of the gravity current to derive power law scaling relationships describing the dissolution and spreading rates in long horizontal aquifers.

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**MS56**

**Using the Immersed Boundary Method to Model Complex Fluid Structure Interaction in Sperm and Ciliary Motility**

Abstract not available at time of publication.

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**MS56**

**Interaction of Vesicles with Fluid and Substrate**

Abstract not available at time of publication.

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**MS56**

**Dynamics of Biofilms**

Abstract not available at time of publication.

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**MS56**

**LBE Model for Non-Newtonian Fluids**

Abstract not available at time of publication.

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**MS57**

**Filtering Random Effects for Array Imaging**

Objects that are buried deep in heterogeneous media produce faint echoes which are difficult to distinguish from the backscattered field. Sensor array imaging in such media cannot work unless we filter out the backscattered echoes and enhance the coherent arrivals that carry information about the objects that we wish to image. I will discuss such filters for imaging in strongly backscattering, finely layered media. The fine layering is unknown and we model it with random processes. The filters use ideas from common seismic imaging techniques, such as normal move-out and semblance velocity estimation. These methods are based on the single scattering approximation, so it is surprising that the filters can annihilate the incoherent echoes produced by random media. I will present a detailed theoretical and numerical study of this phenomenon. I will also show that the filters can be used to estimate the mean sound speed in the medium. Finally, I will present a novel approach for filtering random media effects in more general cases than layered structures.

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**MS57**

**A Level Set Method for Tracking Directional Data**

Tracking directional data such as vectors in a noisy vector field is usually treated as a front propagation problem, which can be erroneous due to local errors or branching of tracks. In this talk we propose a level set based global tracking algorithm which can capture all tracks by using only one single level set function in 2D. The main contribution is the capability of capturing multiple branching tracks without explicit parametrization for each track.

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**MS57**

**Fast Numerical Methods for Electrical Capacitance Tomography (ECT)**

In Electrical Capacitance Tomography (ECT) cross-section images of industrial processes, such as multiphase flows or flame combustion, are reconstructed from fast capacitance measurements, which require no contact with the probe. Mathematically, ECT amounts to a nonlinear inverse problem governed by partial differential equations. We propose and investigate efficient numerical implementations of inversion algorithms for the nonlinear inverse problem, including iterative regularization and sampling methods.

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**MS57**

**Parameter Estimation for Phase Equilibrium Models**

A bilevel program is proposed for parameter estimation in Gibbs free energy models and solved globally with a deterministic algorithm. The reliable prediction of phase equilibria is of extreme importance for the chemical and process industry. Thermodynamic models contain adjustable parameters, which are estimated via phase-split measurements. These measurements typically contain significant noise. Existing parameter estimation methods are inadequate because they use necessary only stability criteria and local optimization. Well- and ill-posed examples are presented.

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**MS58**

**Adaptive Mesh Refinement for Complex Thermal/Fluids Problems**

Adaptive mesh refinement is a powerful tool for augmenting initial mesh generation. We present recent work on goal-oriented adaptivity using adjoints, handling of curved geometry, and grid to grid solution transfer. Examples from multiphysics coupled problems are provided to demonstrate the effectiveness of the adaptive methods.

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**MS58**

**An Optimal Robust Equidistribution Method for Multidimensional Grid Adaptation Based on Monge-Kantorovich Optimization**

We discuss a new multidimensional equidistribution approach for robust grid adapation based on Monge-Kantorovich optimization (MK). The method employs a rigorous constrained minimization approach, and results in a single elliptic nonlinear PDE, which can be solved optimally. A connection between MK and the grid smoothness functional ensures grid quality even in the presence of highly structured Jacobian distributions. In this presentation, we will derive the method, and demonstrate its usefulness with challenging multidimensional examples.

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**MS58**

**Interface Tracking Methods for Multi-material Flows**

Accurate tracking of material interfaces is an important component of multi-material flow simulations such as nuclear reactor cooling, casting, welding and inertial confinement fusion. We will review the different methods for interface tracking namely Volume of Fluid (VOF) methods with Youngs' and LVIRA type reconstruction and Moment of Fluid (MOF). We will then discuss our newly developed material-order-independent interface reconstruction technique in the context of VOF and MOF methods.

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**MS58**

**Common-refinement Based Data Transfer for Multi-physics Coupling**

Multiphysics coupling often requires exchanging data accurately and conservatively between different meshes for different physical domains. In this talk, we give an overview of the common-refinement based data transfer across different meshes, which has been successfully used in a number applications. We present the geometric and topological issues in the construction of the common refinement for meshes with potentially mismatching geometry, the practical issues of robustness and parallel implementation, as well as a comparison with some other conservative data-transfer methods for multiphysics problems.

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**MS59**

**The Numerical Nuclear Reactor**

The Numerical Nuclear Reactor was developed to provide a high fidelity method for light water reactor analysis based on first principles models. High fidelity is accomplished by integrating full physics, highly refined solution modules for the coupled neutronic and thermal-hydraulic phenomena. Each solution module employs methods and models that are formulated faithfully to the first-principles governing the physics, real geometry, and constituents. Specifically, the critical analysis elements that are incorporated in the coupled code capability are a direct whole-core integral neutron transport solution and ultra-fine-mesh computational fluid dynamics/heat transfer solution, each obtained with explicit (sub-fuel pin cell-level) heterogeneous representations of the components of the core. The considerable computational resources required for such highly refined modeling are addressed by using massively parallel computers, which together with the coupled codes constitutes the numerical nuclear reactor (NNR). To establish confidence in the NNR methodology, verification and validation of the solution modules have been performed and are continuing for both the neutronics module and the thermal-hydraulics module for single phase and two-phase boiling conditions under prototypical PWR and BWR conditions. This presentation will describe the features of the NNR, validation of each module, and provides the results of several coupled code calculations.

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**MS59**

**Tightly Coupled Methods for NGNP Reactor Simulation**

There is a growing trend in nuclear reactor simulation to consider multiphysics problems. This can be seen in reactor analysis where analysts are interested in coupled flow, heat transfer and neutronics, These more ambitious simulations usually motivate some level of parallel computing. Many of the coupling efforts to date have been simple code coupling or first-order operator splitting, often referred to as loose coupling. While these approaches can produce answers, they usually leave questions of accuracy and stability unanswered. We are developing a capability to evolved tightly coupled multiphysics tools for nuclear engineering applications. We are utilizing the Jacobian-free Newton-Krylov method along with physics-based preconditioning. We are also leveraging a significant level of previously developed software in order to build the Multiphysics Object-Oriented Simulation Environment (MOOSE). MOOSE is then used to rapidly develop other multiphysics application codes. In this presentation we will present models and methods in PRONGHORN, our 3-D coupled flow, heat transfer, and neutronics code for pebble bed gas cooled reactors.

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**MS59**

**High Resolution Multiphysics Simulations of Z-Pinch with ALEGRA**

To successfully simulate the implosion of wire-arrays with SNLs Z-Machine many physical processes must be included integrated simultaneously. Key among these is the close coordination of hydrodynamic, magnetic and radiation transport. Each of these processes produces essential aspects of the observed physical effects. Moreover, the demands on the quality of the numerical method are profoundly greater than other comparable systems. Here the steps taken to allow our simulations to achieve their observed quality are detailed

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**MS59**

**Implict Compressible Flow Methods for NGNP Reactor Simulation**

This talk is intended to present the initial performance of an implicit fully-coupled Newton-Krylov based solver applied to a simplified NGNP reactor flow problem. The study will consider Boussinesq, low Mach number and compressible flows with the governing PDEs discretized by unstructured stabilized finite element methods. The Krylov linear solver is preconditioned by an algebraic multilevel technique that employs a graph-based aggressive-coarsening aggregation method that uses the nonzero block structure of the Jacobian matrix..

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**MS60**

**Inverse Transport Problems**

Inverse transport consists of reconstructing optical parameters from boundary measurements. Several types of measurements may be considered depending on technological feasibility: one may either perform angularly resolved or angularly averaged measurements. One may also perform time dependent measurements or steady-state measurements. I will present recent results showing which parts of the optical parameters may be reconstructed in a stable fashion under these measurement scenarios. I will then show how these results degrade in the presence of physical

noise.

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**MS60**

**Phase Approximation for Bioluminescence Tomography**

By approximating the phase function in the radiative transfer equation (RTE) as a generalized delta-Eddington phase function, we have developed a phase approximation (PA) model to solve the RTE effectively and efficiently. Based on the PA model, here we report inverse algorithms for estimation of the optical properties and reconstruction of the bioluminescent source distribution inside a living mouse. Our data show a superior imaging performance as compared to that of the popular diffusion approximation (DA) model.

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**MS60**

**The Inverse Source Problem In Bioluminescence Tomography**

Bioluminescence tomography recovers the spatial distribution of light-emitting reporter probes in highly scattering small animal tissue by solving an inverse source problem. A light transport model based on the simplified spherical harmonics equations is numerically solved and its solutions are used for building an iteration matrix. Iterative inversion of the matrix leads to a solution for the sought source distribution for a given partial boundary flux on the tissue surface.

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**MS60**

**A Fast Forward Solver for Radiative Transfer Equation**

I will present an efficient forward solver for steady-state RTE on both structured and unstructured grid. We develop a Gauss-Seidel iterative scheme that incorporates dominant scattering and angular dependent ordering effectively. The iterative method is then used naturally as an efficient relaxation scheme for multigrid solver in both spatial and angular space. I will demonstrate both efficiency and accuracy of our forward solver by extensive tests and applications in various optical imaging regimes.

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**MS61**

**Through the Mathematical Looking Glass: Achievements, Challenges, Perspectives in Cancer Modelling**

Recently a new breed of mathematical model has emerged, and with it new computational approaches - some of which were presented within this mini-symposia. What have we achieved with these approaches, how can we balance complexity with understanding and ultimately what impact can we have on the complex multiscale evolving system that is Cancer? I will discuss these issues within the context of my own experience in working with biologists testing models of tumor invasion.

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**MS61**

**Multiscale Modeling of Cell-stroma Interactions in Tumor Angiogenesis**

We have developed a multiscale modeling framework and applied to study tumor angiogenesis. Our model incorporates the subcellular signaling pathways, cellular level cell growth and division, cell-cell and cell-stroma interactions, as well as tissue level dynamics. I will present our recent results on cell-stroma interactions. In particular, I will focus on the effects of angiogenic factor, VEGF, and the topography of extracellular matrix, on sprout morphogenesis.

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**MS61**

**Multiscale Models of Solid Tumor Growth and Angiogenesis**

In this talk, we discuss recent efforts in multiscale modeling of solid tumor growth and angiogenesis. We apply a biologically founded, multi-scale, mathematical model to identify and quantify tumor biologic and molecular properties relating to clinical and morphological phenotype and to demonstrate that tumor growth and invasion are quantifiable processes governed by biophysical laws, and regulated by heterogeneity in phenotypic, genotypic, and microenvironmental parameters, including the neovasculature. This heterogeneity drives migration and proliferation of emerging more aggressive clones up cell substrate gradients within and beyond the central tumor mass, while often also inducing loss of cell adhesion. The model predicts that this process triggers a gross morphologic instability that leads to tumor invasion via cell chains, strands or detached clusters infiltrating into adjacent tissue producing the typical morphologic patterns seen, for example, in the histopathol-

ogy of glioblastoma multiforme.

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**MS61**

**Computational and Experimental Models of Tumor Angiogenesis**

Multiscale computational models of angiogenesis will be presented that include molecular-detailed equation-based models of hypoxia-inducible factor (HIF), vascular endothelial growth factor (VEGF), and matrix metalloproteinases (MMPs), as well as agent-based model of capillary sprouting and neovascular network formation. The model of VEGF is extended from molecular to whole body level and is applied to investigate administration of a VEGF-neutralizing molecule as antiangiogenic anticancer therapeutic. Computational results are compared to animal experiments.

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**MS62**

**Progress in Adaptive Construction of Master Equation Models and Application to Laser-induced Temperature-jump Kinetics for the Trpzip2 Peptide**

Discrete-state Markov models are emerging as a powerful way to describe the statistical dynamics of biological macromolecules. Here, we discuss methodological advances and steps toward application of the method to describe the observed laser-induced temperature jump relaxation spectra of the trpzip2 peptide, a system that has been well-characterized experimentally by a variety of spectroscopic means.

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**MS62**

**Coarse-graining and Sampling of Markov Propagators and Generators and their Application to Modeling Protein Folding**

Methods will be presented to compute the essential dynamics of complex metastable systems from Markov propagators or generators with application to protein folding. This includes:

1. Coarse-Graining of the original Markov propagator or generator to metastable sets
2. Computing of transition pathways between subsets of the state space
3. Estimation of Errors of properties of the coarse-grained description
4. Application to molecular dynamics simulations of protein folding

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**MS62**

**Hierarchical Refinement in Conformation Dynamics**

Whenever the stationary density of molecular dynamical systems decomposes into almost invariant partial densities, its computation from long-time dynamics simulations is infeasible due to the well-known "trapping problem'. To avoid this computational difficulty, we suggest a domain decomposition approach that is similar to umbrella sampling methods. In contrast to standard techniques, our decomposition forms a partition of unity such that the corresponding stationary density can be computed as eigenvector of some mass matrix.

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**MS62**

**Comparing Different State Decompositions for Molecular Dynamics Simulations**

Markovian state models represent the dynamics of a molecular system as Markovian transitions between discrete conformational states. Defining the states in this model is difficult, and poor state definitions can lead to non-Markovian behavior. In this presentation, we discuss new Bayesian scoring techniques which compare state decompositions that differ in the definitions and the number of states. These techniques are more discriminative than previous methods for comparing state decompositions.

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**MS63**

**Recent Work on AMR for ALE Hydrodynamics**

Arbitrary Lagrangian Eulerian (ALE) methods combined

with adaptive mesh refinement (AMR) focuses computational resources in specific regions while allowing grids that move and adapt to the flow, joining the advantages of ALE methods with the added efficiency of AMR. Our recent work has focused on implementation of ALE/AMR in existing multi-physics codes. Some issues we discuss in this talk include code verification, strength of materials, and parallel scalability.

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**MS63**

**Adaptivity and Scientific Computing: From von Neumann to the Stars**

Adaptivity is at the core of all modern computational methods, from the adaption of the solution method to the flow, to refinement schemes for enhanced resolution. This talk outlines some history of adaptivity in compressible flow solution. These include the early artificial viscosity methods of von Neumann, the development of multi-dimensional Lagrangian hydrodynamic methods, high-order Eulerian Godunov schemes and the rise of adaptive mesh refinement as a scheme of choice for high resolution flows.

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**MS63**

**Subgrid Models for Mass and Thermal Diffusion in Turbulent Mixing**

We investigate chaotic mixing in reshocked Richtmyer-Meshkov unstable flows. We seek converged solutions for macro solution features like mixing zone edges and micro solution features for the joint probability distributions of temperature and species concentration. Parameterized subgrid models of mass and thermal diffusion define LES that replicate the micro features observed in the DNS. We explore the variation of the Schmidt, Prandtl and Reynolds numbers by three orders of magnitude in DNS and LES regimes.

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**MS63**

**Adaption of Direct Eulerian Flow Solvers for Three Temperature Plasma Physics**

The evolution equations for electron and ion specific internal energies in a three temperature plasma physics model contain nonconservative products, which require careful numerical treatment. Assuming isentropic discontinuities in electron quantities at shocks permits semi-analytical solutions for simple flows that exhibit differential shock heating of electrons and ions. We have adapted an Eulerian Godunov-based scheme to compute such shocks. We provide details of the numerical scheme and compare the computed and semi-analytic solutions.

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**MS64**

**Finite Element Methods for a Polymer Gel Model**

Abstract not available at time of publication.

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**MS64**

**Numerical Simulation of Inhomogeneous Flows of Flowing Polymer-particulate Nanocomposites**

Abstract not available at time of publication.

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**MS64**

**Motors Based on Shape Change: See How They Run**

Motors are devices which produce motion due to the transfer of energy, but not of momentum. Recent advances in materials science have allowed the construction of motors where the motion is produced via changes in the shapes of solid objects. In this talk, we consider motors where the shape change is a bend, rather than an elongation/contraction. We analyze in detail of the mechanisms which bring about the motion, and discuss the origins and path of the momentum current which is generated. We present the results of numerical simulations, and compare these with experimental observations.

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**MS64**

**One Order Parameter Tensor Mean Field Theory for Biaxial Liquid Crystals**

In this talk, we present a simple one tensor mean field model of biaxial nematic liquid crystals. One unusual feature of our approach is that physical parameters appear explicitly in our order parameter tensor. We construct the free energy from explicit intermolecular interactions, and obtain self-consistent equations, which are then solved numerically. We examine the resulting phase diagrams, discuss the relation between one- and two order parameter tensor models, provide a Landau expansion and discuss the relation between molecular parameters and the stability of the biaxial phase. We identify the underlying common aspects of one- and two-order parameter models and Landau and molecular theories.

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**MS65**
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**MS65**
**Stochastic Data Assimilation, Multiscale Modeling, and Model Validation**

We describe procedures for stochastic data assimilation which include adaptations of particle filtering, maximum entropy, and maximum likelihood methods. We highlight the relationship between the dimensionality of the ensuing polynomial chaos representations and the concepts of model sufficiency and validation, and the natural multiscale interpretation of these representations.

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**MS65**
**A Stochastic Newton Method for Bayesian Inverse Problems**

We present a new MCMC method for sampling high-dimensional, expensive-to-evaluate probability density functions. We improve upon Langevin sampling by using local Hessian information to guide sampling, drastically improving acceptance probabilities and MCMC convergence rates. The resulting method resembles a stochastic variant of Newton's method. We demonstrate by solving a statistical inverse problem governed by 1D seismic wave propagation with up to 65 parameter dimensions, for which the new method is two orders of magnitude faster than conventional MCMC.

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**MS65**
**Stochastic Collocation for Bayesian Inference in Inverse Problems**

We present an efficient numerical strategy for the Bayesian solution of inverse problems. Stochastic collocation methods, based on generalized polynomial chaos (gPC), are used to construct a polynomial approximation of the forward solution over the support of the prior distribution. This approximation defines a surrogate posterior probability density that can be evaluated repeatedly at minimal computational cost. We prove convergence of the approximate posterior to the true posterior and obtain an estimate of the convergence rate, then demonstrate the scheme on nonlinear inverse problems of varying smoothness and dimension.

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**MS66**
**Improving ALE Applications via Optimization-based Smoothing Techniques**

ALE applications have complex requirements for mesh quality improvement tools including the need for low cost element shape improvement that constrain vertex movement to preserve mesh characteristics, numerical accuracy and stability. In this talk, we describe our experiences with using Mesquite to improve KULL application meshes including the interaction between application limiters and Mesquite, the parallel algorithms needed for in-situ use of Mesquite, and how our results compare, both in terms of speed and effectiveness, with the currently used equipotential smoother.

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**MS66**
**A Mesh Optimization Algorithm to Decrease the Maximum Error in Finite Element Computations**

We present a mesh optimization algorithm for adaptively improving the finite element interpolation of a function of interest. The algorithm minimizes an objective function by swapping edges and moving nodes. Numerical experiments are performed on model problems. The results illustrate that the mesh optimization algorithm can reduce the $W^{1,\infty}$ semi-norm of the interpolation error. For these examples, the $L^2$, $L^\infty$, and $H^1$ norms decreased also.

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**MS66**
**Smoothing Mesh Boundaries with Mesquite**

Mesquite has been shown to be highly effective at improving mesh quality by moving vertices using optimization-based techniques. However, it is often necessary to constrain the movement of boundary vertices to preserve material or domain boundaries. We describe a new algorithm built on the Mesquite infrastructure that smoothes boundary vertices such that arbitrary polyhedral material or domain boundary surfaces are preserved. Several examples of its use on complex geometries defined by CAD systems

and for internal material interfaces are given.

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**MS66**

**Efficiency of Static Vertex Reordering Schemes for Local Mesh Optimization**

Finite element meshes and their quality can greatly impact the accuracy of PDE simulations. Smoothing can be used to improve the mesh quality; a common technique is the local-patch method which smoothes one patch at a time. In this study, we examine the effect altering vertex ordering has on the CPU time to achieve the desired quality level with the goal of convergence acceleration. Results indicate several successful vertex reordering strategies for local mesh optimization.

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**MS67**

**Smoothed Aggregation and Algebraic Multigrid Methods for Markov Chains**

Two multilevel methods for the numerical calculation of the stationary probability vector of large sparse irreducible Markov chains are presented. The first method uses smoothed aggregation, and the second uses algebraic multigrid. A lumping technique assures well-posedness of the coarse-level problems, leading to positivity of the probability vector solution on all coarse levels. Numerical results show that these methods lead to nearly optimal multigrid efficiency for a representative set of test problems.

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**MS67**

**Least-squares Based Multilevel Eigensolvers for Markov Chain Applications**

To guarantee efficient performance of algebraic multilevel methods for solving the eigenproblem $Bx = x$ in Markov Chain applications, we are using an adaptive setup that captures the nature of the eigenmode of interest. The least-squares based approach computes appropriate test-functions and fits them to define highly accurate interpolation that leads to a robust multilevel performance. The current algorithm's implementation is based on the smoothed aggregation approach, but can be generalized to arbitrary grid hierarchies.

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**MS67**

**On Optimal Smoothing Parameters in Smoothed Aggregation Multigrid for Markov Chains**

Recently, smoothed aggregation multigrid algorithms were developed to compute the steady-state eigenmode of stochastic matrices with scalable computational complexity. A lumping technique ensures well-posedness of coarse-grid problems in the multilevel hierarchies. This work discusses the choice of parameters for smoothing interpolation and restriction operators with the goal of minimizing the amount of lumping required for well-posed coarse-grid problems. A trade-off between optimal smoothing and lumping is discovered and addressed.

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**MS67**

**Square and Stretch Multigrid for Stochastic Matrix Eigenproblems**

A novel multigrid algorithm for computing the principal eigenvector of column stochastic matrices is developed. The method is based on the *Exact Interpolation Scheme* multigrid approach of Brandt and Ron, whereby the prolongation is adapted to yield a better and better coarse representation of the sought eigenvector. The main novelty of the present approach is in the squaring of the stochastic matrix - followed by a stretching of its spectrum - just prior to the coarse-grid correction process. This procedure is shown to yield good convergence properties, even though a cheap and simple aggregation is used for the restriction and prolongation matrices, which is essential for maintaining competitive computational costs. An additional contribution of this paper is a novel bottom-up procedure for defining the coarse-grid variables.

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**MS68**

**Outside-in Uncertainty Quantification for Hard Black Boxes**

How should we project uncertainty through black-box models when their computational complexity restricts how many sample realizations can be evaluated? We suggest approaches that estimate the uncertainty conservatively but that become tighter as the total computational effort increases. Such an outside-in approach to quantifying uncertainty can be used for deterministic models, for probabilistic models capturing aleatory uncertainty, for models with epistemic uncertainty characterized by intervals, and for mixed models with both forms of uncertainty.

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**MS68**

**Model Validation and Predictive Capability**

A validation metric is proposed that can be used to characterize the disagreement between the probabilistic predictions from a model and relevant empirical data. The metric can be used to estimate model accuracy when the model is used to extrapolate to conditions for which direct experimental observations are not available. Using a simple example problem, we compute the validation metric and show how it can be used in predictive capability.

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**MS68**

**Overview of Verification, Validation, and Uncertainty Quantification in Scientific Computing**

Verification, Validation, and Uncertainty Quantification (VV&UQ) are a formal set of procedures for assessing the predictive capability of models in scientific computing. This talk will begin by providing a broad overview of the VV&UQ process from both the deterministic and nondeterministic points of view. It will conclude with a more detailed discussion of the role of verification in assessing the predictive capability of simulations.

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**MS68**

**A Posteriori Error Estimates of the Discontinuous Galerkin Method for Symmetrizable Hyperbolic Systems**

*A posteriori* error estimates are a useful tool to verify the quality of finite element approximations and to control the error in adaptive meshes. We apply the Discontinuous Galerkin Method to first-order linear symmetrizable hyperbolic systems in two and three space dimensions. We explicitly write down the leading error term and solve local finite element problems to obtain a *a posteriori* error estimates. We present convergence and numerical results for problems from acoustics and electromagnetism.

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**MS69**

**Simulating Tsunamis in the Indian Ocean with Real Bathymetry by Using a High-order Triangular Discontinuous Galerkin Oceanic Shallow Water Model**

The discontinuous Galerkin (DG) method has come into prominence in the last decade in all areas of numerical modeling and especially in the last few years has received attention in geophysical fluid dynamics. The high-order accuracy, geometric flexibility to use unstructured grids, local conservation and monotonicity properties of the DG method make it a prime candidate for the construction of future ocean and shallow water models. In this presentation we will show the exponential convergence of the model by using analytic solutions of the two-dimensional shallow water equations using the linear Stommel and Munk problems; this convergence study is facilitated by having analytic solutions to these problems. In addition, we will show error norms of our model with analytic solutions to shallow water flow with bathymetry. Finally, using real bathymetry data of the Indian Ocean we will simulate the Indonesian Tsunami of 26 December 2004 and validate this

simulation by using real measurements.

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**MS69**

**Sierpinski Curves and Recursively Structured Adaptive Grids for Tsunami Simulation**

Efficient adaptive refinement, to capture land-ocean boundaries to model inundation and to dynamically refine along propagating wave-fronts, is a performance-critical component of Tsunami simulation. We present an approach to the numerical simulation of dynamically adaptive problems on recursively structured adaptive triangular grids, which are sequentialised in memory using Sierpinki space-filling curves. This leads to a storage scheme that requires only a minimal amount of memory and allows adaptive simulations with several million grid cells and mesh refinement and coarsening in each time step. Test results are demontrated for a Discontinuous Galerkin solver for the shallow water equations.

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**MS69**

**Development of an Unstructured Adaptive Grid Tsunami Propagation and Inundation Model**

In simulating tsunami propagation and inundation behavior, non-linear shallow water codes with special wetting and drying algorithms along the land boundaries have proven their accuracy and reliability. Especially unstructured triangular mesh based numerical schemes have been successful in accurately resembling measured tsunami inundation behavior. However, for high local accuracy, mesh resolutions of 100 m or less are required. Together with a necessary extent of the computational domain of thousands of kilometers (a whole ocean basin) computational demands quickly exceed available resources. An adaptive mesh refinement strategy combined with a stable and accurate finite element discontinuous discretization scheme has been developed to provide tsunami simulation capabilities beyond currently existing methods. Thorough validation as well as performance optimization is required to make these developments accessible to the tsunami simulation community.

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**MS69**

**Adaptive Mesh Refinement for Tsunami Modeling**

Tsunami waves on the deep ocean have a wavelength of several hundred kilometers, requiring only a moderate grid resolution, while fine-scale local features in the bathymetry and topography near the shoreline can dramatically influence inundation patterns. One is often interested in modeling features on the scale of a few meters near shore, which is impossible without adaptive mesh refinement (AMR). This application presents several unique mathematical and computational challenges in the development of AMR methods that will be discussed in this talk.

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**MS69**

**Tsunamis from Asteroid Impacts in Deep Water**

Oceans cover three-quarters of the Earth's surface, yet geological evidence for deep ocean impact events is scarce. Tectonic subduction has wiped away essentially all of the oceanic crust that is older than 150 million years, and most of the seafloor crust that remains is still very poorly mapped. Moreover, water soaks up so much of the energy of an impacting meteor that persistent craters form only in shallow-water impacts. Tsunamis are virtually the only signature of deep-water impacts. We have performed a large number of numerical calculations of deep-water impacts to understand energy deposition and tsunami generation from these events. These are done in two and three dimensions with the multi-material adaptive-mesh hydrocode Sage. We will discuss results for impactors of various compositions and sizes from 100 m to 5 km diameter, and compare the expectations with the geological record. The kinetic energy per unit mass of a typical meteor is very much larger than the latent heat of vaporisation of water, and most of the total free energy is immediately carried away into the atmosphere by the explosively expanding vapour cloud. Of the remaining energy, a substantial portion is used in the crown splash and the rebound jet that forms as the transient crater collapses. A small fraction of the energy remains for the generation of a high-amplitude wave of intermediate length (shorter than typical tsunamis) that tends to break in the open ocean, and doesn't propagate efficiently over long distances. Impacts in this size range are inefficient generators of long-wavelength teletsunamis, though the crown splash and initial waves for impacts that occur close to shore could be dangerous and leave lasting signatures.

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**MS70**

**The Reactive Riemann Problem for Thermally Perfect Gases**

We investigate the reactive Riemann problem for thermally

perfect gases as the reactive shock is in deflagration or detonation regime. Indeterminacy of deflagration regime is removed imposing the fundamental flame speed of the reactive shock. An iterative algorithm is proposed for the solution of reactive Riemann problem and is also used to design an approximate reactive Riemann solver. Numerical experiments here presented show that the proposed algorithm is robust at all combustion regimes.

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**MS70**

**The Soret Effect and Hydrogen Flames at the Flammability Limit**

Abstract not available at time of publication.

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**MS70**

**Combustion Modeling in Safety Analysis for Large-scale Industrial Objects**

In the current work several models for the slow to fast flames and for the transition from quasi-laminar to fast deflagration are discussed. Particular attention is paid to the interaction between combustion and turbulence models. Finally the current state of models development is illustrated presenting simulations for different industrial objects ranging from medium scale under-expanded jet to very large hydrogen release into open atmosphere.

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**MS70**

**The Deflagration-to-Detonation Transition: Turbulence, Hot Spots, and Stochasticity**

Multidimensional, unsteady, reactive numerical simulations have taught us how flames develop, spread, become unstable, interact with shocks, and undergo transition to detonations. Here we first describe simulations of flames propagating in hydrogen-air mixtures and then use these to discuss the effects and generation of turbulence, the formation of reaction gradients and spontaneous waves, and the effects of stochastic processes on our ability to predict the properties of such and dynamic systems.

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**MS71**

**Recycling BiCG for Model Reduction and Other Applications**

Engineering problems frequently require solving a sequence of large linear systems. This paper presents a modified Bi-CG that recycles Krylov subspaces from one linear system to the next. The recycle spaces are approximate left and right invariant subspaces found by solving a sequence of small generalized eigenvalue problems while solving a linear system. Augmented bi-Lanczos and modified two term recurrence are developed for using the recycle space. The theory for using a recycle space is extended to CGS. Experiments on model reduction problems show promising results.

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**MS71**

**Solving Sequences of Linear Systems - An Overview**

We give an overview of techniques for improving the convergence of iterative linear solvers with some emphasis on solving sequences of linear systems arising in time-dependent problems, nonlinear systems of equations, and optimization. We demonstrate the effectiveness of these techniques with results from several relevant applications.

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**MS71**

**Multiple Right-hand Side Systems with Application to QCD**

We will discuss Krylov iterative methods for solving systems of linear equations with multiple right-hand sides. The methods will involve deflation of eigenvalues. Eigenvector information developed while solving the first right-hand side essentially removes small eigenvalues from the solution of subsequent right-hand sides. These methods compete with block methods, but possibly can also be useful along with block approaches. We will give methods for both symmetric and nonsymmetric problems and will use a seed conjugate gradient method and deflated restarted Lanczos and GMRES. Application will be given to large Hermitian and non-Hermitian problems from lattice quantum chromodynamics (QCD).

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**MS71**

**Extending EigCG for Computing Eigenpairs While Solving Linear Systems to the Nonsymmetric Case**

Recently we have presented eigCG, an extension to the CG method, that computes eigenvectors and eigenvalues from a restarted window of the CG residuals. The window is restarted with a combination of thick and LOBPCG-type restarting, but the CG iteration for solving the linear system is unaffected. Surprisingly, eigenpairs converge similarly to unrestarted Lanczos. We present an extension of eigCG to eigBICG for nonsymmetric matrices with equally surprising and successful results. We also present an efficient way to deflate approximate eigenvectors.

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**MS71**

**Various Ways to Use a Second Level Preconditioner**

In many applications, preconditioned Krylov methods are used to solve large sparse linear systems. A good preconditioner is very important to obtain a fast and robust solver. Many good preconditioners are known which are based on ILU, multi-grid, approximate inverse, domain decomposition, etc. However for difficult problems a number of *bad* eigenvalues can spoil the convergence. This motivates the development of second level preconditioners. These preconditioners are made such that the *bad* eigenvalue components are removed from the error and residual. There are various ways to include a second level preconditioner. There are methods based on deflation, recycling, multi level or domain decomposition approaches. In this presentation we try to give a general preconditioned CG method such that many variants fit into this algorithm. We summarize a number of theoretical results in order to compare the different variants. It appears that not only theory is important also the implementation, rounding errors, termination criteria can play an important role. We show the effect of these issues on the various second level preconditioners by numerical experiments. It appears that these comparisons leads to guidelines how to choose the best method for a certain application.

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**MS72**

**Numerical Methods for Inverse Diffusive Optical Tomography**

Light in the red and infrared range propagates in biological tissues with little attenuation but is frequently scattered. It can therefore be used to probe the optical properties, for example for tumor detection, but the diffusive nature of the medium yields a very ill-posed inverse problem. This talk will address the resulting challenges for efficient and accurate numerical methods to solve such problems at realistic scales

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**MS72**

**Optical Tomographic Imaging with PDE-constrained Algorithms**

It is well known that transport-theory-based reconstruction algorithms provide the most accurate reconstruction results in optical tomographic imaging. However, these codes require large amounts of memory and are usually slowly converging. To overcome theses problems we have developed algorithms that employ PDE-constrained methods. We have evaluated the performance of various PDE-constrained schemes with numerical and experimental data and have found that the computation and memory requirement can be considerably reduced without affecting the accuracy of the solutions.

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**MS72**

**Transport Based Fluorescence Optical Tomography with Multi-frequency Measurements**

Diffusion theory based image reconstruction algorithms for near infrared optical tomography are not accurate for molecular imaging in small animal volumes, where source-detector separations are limited, and absorption in the internal organs is not negligible compared to scattering. We have implemented a radiative transport based transport modeling approach for small animal fluorescence optical tomography which provides rapid solution on arbitrary animal geometries for non-contact measurements. We will present the results on the coupling of the developed transport algorithm with a multi-modality and multi-frequency mice imaging instrumentation setup

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**MS72**

**An Inverse Source Problem for the Vector Radiative Transport Equation**

We study the light that exits a halfspace composed of a uniform absorbing and scattering medium due to an unpolarized, isotropic, and continuous planar source. Using only angular integrals of the two orthogonal components of the intensity exiting the halfspace, we recover the depth and strength of this source. This method is limited to sources located at depths on the order of a transport mean-free path or less. Numerical results to validate this method.

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**MS72**

**Uncertainty Quantification In Transport-Based Biomedical Imaging**

In this talk, we report a numerical procedure based on a preconditioned Markov Chain Monte Carlo method for uncertainty quantification in transport-based optical tomography and optical molecular imaging. We show that by using approximate transport solutions (from either truncated Neumann series or diffusion approximations), we can accelerate the Monte Carlo simulation significantly. Numerical results on synthetic data will be presented to demonstrate the efficiency of the method.

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**MS73**

**Toward Optimal Transport Networks**

Strictly evolutionary approaches to improving the air transport system - a highly complex network of interacting systems - no longer suffice in the face of demand that is

expected to double or triple by 2025. It is necessary to arrive at active design methods. The ability to actively design, optimize and control a system presupposes the existence of predictive modeling and reasonably well-defined functional dependencies among the controllable variables of the system and objective and constraint functions for optimization. We investigate functional relationships that govern the performance of transport networks with the aim of arriving at substantiated modeling, design, and control methods.

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**MS73**

**Uncertainty Quantification as a Tool for the Validation of Computational Models**

Validation is a rigorous process for building confidence in the predictive capability of a model, and UQ is one of the fundamental tools in executing this process. In particular, it brings statistical rigor to the analysis of both computational and experimental data and the comparison between the two. In this talk, we will present some specific examples of the execution of a UQ study for physics-based simulators.

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**MS73**

**Fuzzy Decision Analysis of Bug Escapes in a Product Life Cycle**

Bugs (or design defects) are generated at every stage of a typical product lifecycle. Focusing on chip development and production stages in the semiconductor industry, we present both the forward and backward problems of bug escapes. In the forward problem, we examine how expert (subjective) bug categorization and consequent decisions affects downstream actions, schedules, and product quality. In the backward problem, we examine customer excursions and tie these back to upstream events.

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**MS73**

**Recent Advances in Markov Chain Monte Carlo Sampling and Particle Filtering for Uncertainty Quantification in Nonlinear Models**

Markov chain Monte Carlo and Particle Filtering have found widespread use in many fields of study for posterior inference and tracking. In this talk, I will highlight computationally efficient, user-friendly implementations of these methods using recent advances in differential evolution Markov Chain sampling. I will demonstrate these developments using a classical rainfall runoff example, and three-dimensional flow and transport modeling using Magnetic Resonance Imaging (MRI) data of a conservative tracer moving through a flow cell. This work is in collaboration with Cajo J.F. ter Braak, Cees G.H. Diks, and Ming Ye

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**MS74**

**Using Nonnegative Tensor Factorization for Scenario and Plot Discovery**

The expanding field of visual analytics requires automated approaches for the verification and discovery of scenarios and plots defined by the behaviors and actions of primary actors through time. Data mining and knowledge discovery play critical roles in facilitating the ability to extract semantic information from large and somewhat unstructured textual-based media. In this study, we demonstrate a prototypical scenario discovery software platform called TGIST (Tensor Group Interactive Summarization Tool) that uses a variant of the PARAFAC multi-way data model to extract and sequence related activities andspecific events from tagged or untagged information sources. The ability to automatically reconstruct a plot or scenario from the visualization of model outputs is a primary goal of TGIST. Nonnegative tensor factorization (NTF) is used within TGIST to expose the terrorism-based scenarios of the VAST 2007 and 2008 Contest data sets to demonstrate how term-by-entity associations can be used for scenario/plot discovery and evaluation.

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**MS74**

**Low Rank Orthogonal Approximation of Tensors**

Standard approximations of tensors include the Tucker and the Parafac models. This talk presents an alternative called the Low Rank Orthogonal Approximation of Tensors (LROAT), which consists of a linear combination of rank-1 tensors satisfying orthogonality constraints. In contrast with the Parafac model, an optimal solution is guaranteed to exist (under a rank condition). Moreover, LROAT is equivalent to a tensor decomposition which maximizes the diagonal of the core tensor. An algorithm to compute the LROAT approximation is presented.

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**MS74**

**A New Factorization of an Order-$p$ Tensor as a**

**Product of Order-$p$ Tensors**

The standard model extending the SVD to higher-order tensors involves the outer product. Here, we present a new higher-order generalization of the SVD where an order-$p$ tensor is instead decomposed as a *product* of order-$p$ tensors. New definitions then result such as the tensor transpose, inverse, and identity. A major motivation for developing tensor multiplication is to devise new types of factorizations for tensors which could then be used in applications such as data compression.

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**MS74**

**A Parallel Algorithm for Approximate Nonnegative Tensor Factorization**

Given the rapid data collection in various research areas, large dataset processing using tensor methods typically demands faster computers with larger memories. DNA sequence data on a sample of several thousands, for example, could yield a matrix of order thousands to millions. A large dataset of global climate data collected by NASA (and used in this study) constitutes $720 \times 360 \times 252$ values for each parameter, including temperature, precipitation and barometrics. Combining those parameters would yield a data matrix of order comparable to the DNA data. Given these large datasets, implementing methods like Nonnegative Matrix Factorization (NMF) or Nonnegative Tensor Factorization (NTF) on a single processor computer would be quite slow and implementing them on a System-On-Chips (SOC) platform would be even more challenging, if not impossible. One approach, for example in genetics study, is to de-correlate data at distant parts and thus to treat the small chunks of data sequentially, which is certainly faster and saves memory at the risk losing certain traits that express at distant parts of the data. Our approach would inherent the global nature of NMF and NTF, but parallelize the algorithms through certain understandings of the matrices used in the process. Specifically, the core NMF problem uses only a much smaller quadratic form of component matrices, rather than component matrices themselves. Much memory and time are spent on computing these quadratics using a single thread with preloaded matrices and thus if parallelized, savings would be immediate. This also opens up the possibility of implementing it on a SOC platform. We also pipeline the algorithms by splitting the original dataset and parallel processing each section but combine in the end. This enables us to process arbitrary large datasets with limited memory, but without de-correlation, while most current approaches usually load the whole dataset into memory firsthand. We will demonstrate this using our parallelized NTF method on the combined NASA climate dataset with emphasis on computation complexity and time.

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**MS75**

**Systems Biology for the Petascale: Simulation and Optimization of Cellular Metabolism**

Metabolic engineering is an important discipline for improving bioenergy production. We describe the parallel software **HiPer SBTK**, a toolkit to simulate, fit, and optimize metabolite concentrations and fluxes with respect to enzyme kinetic parameters and concentrations in a thermodynamically formulated metabolic network. Critical to forward time integration, sensitivity analysis and optimization are the calculation of time derivatives, Jacobians, and Hessians. The advantages and disadvantages of AD approaches from our perspective as users will be discussed.

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**MS75**

**ColPack: A Graph Coloring Package for Sparse Derivative Computation**

Large and sparse derivative matrices can be computed *efficiently* and *accurately* via automatic differentiation (AD) using the following four-step procedure: determine the sparsity pattern of the derivative matrix $A$ using AD; using an appropriate coloring on a graph representation of the sparsity pattern, obtain a seed matrix $S$; compute the compressed matrix $B \equiv AS$ using AD; and recover the numerical values of the entries of $A$ from $B$. ColPack is a software package consisting of implementations of a variety of algorithms for the second and the fourth step. We discuss the functionalities available in and the organization of ColPack.

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**MS75**

**Optimal Dynamic Operation of Simulated Moving Bed Processes in Chemical Engineering**

Simulated moving bed (SMB) chromatography has been widely used in many industries for over 40 years. In recent years, it has been gaining attention in the pharmaceutical industry as an efficient production technique. In this presentation, systematic approaches for optimizing the SMB operation are discussed. The dynamic optimization problem is discretized to create a large scale nonlinear optimization problem, and it is solved by utilizing exact first and second derivatives obtained by automatic differentiation.

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**MS75**

**Automatic Differentiation via Operator Overloading: The ADOL-C Tool**

After a short introduction to Automatic Differentiation (AD), we discuss related implementations strategies based on operator overloading by means of the AD-tool ADOL-C. ADOL-C is designed for the differentiation of C and C++ codes and can handle classes, templates and other advanced C++-features. Recent developments, including the treatment of iterative processes and parallel function evaluations, are discussed. Finally, some examples covering aerodynamics and the computation of quantum-plasma illustrate the potential of ADOL-C.

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**MS76**

**Viscoelastic Fluid-structure Interactions**

Abstract not available at time of publication.

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**MS76**

**On the Yield Stress of Fiber Reinforced Plastic Materials**

Abstract not available at time of publication.

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**MS76**

**Kinetic Simulations of Flowing Nematic Liquids in Confined Geometries**

Abstract not available at time of publication.

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**MS77**

**Particle Kalman Filtering and Data Assimilation in Meteorology and Oceanography**

This contribution discusses a new approach to tackle the optimal nonlinear filtering problem in meteorology and oceanography, called particle Kalman filter (PKF). The PKF is based on a local linearization in a kernel representation of the state's probability density function. This leads to a discrete nonlinear filter in which the standard (weight-type) particle filter correction is complemented by a Kalman-type correction for each particle using the covariance matrix of the kernel mixture. The solution of the nonlinear filtering problem is then obtained as the weighted average of several Kalman filters operating in parallel. The Kalman-type correction reduces the risk of ensemble degeneracy, which enables the filter to efficiently operate with fewer particles than the particle filter. Running an ensemble of Kalman filters is, however, computationally prohibitive for high dimensional systems. This contribution discusses approaches to reduce the computational burden of the PKF filter suitable for atmospheric and oceanic data assimilation problems. First the popular ensemble Kalman filter is derived as a simplified variant of the KPF. Then simplified Particle Kalman Filters are introduced and their performances compared with a Lorenz model.

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**MS77**

**Efficient Uncertainty Prognostic Schemes for Physical, Acoustical, and Biogeochemical Fields in the Ocean**

Abstract not available at time of publication.

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**MS77**

**On Numerical Properties of Particle Filter**

Particle filter is one of the most widely adopted filtering methods for sequential data assimilation in complex systems. Also termed "sequential Monte Carlo method", it is a kind of recursive Bayesian filter based on Monte Carlo simulation. In this talk we present a rigorous estimate of numerical error of particle filter. We establish the convergence of particle filter and focus on the effect of assimilation step size on the error behavior.

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**MS77**

**Particle Filtering with Path Sampling and an Application to a Bimodal Ocean Current Model**

I will introduce a recursive particle filtering algorithm designed to filter high dimensional systems with complicated non-linear and non-Gaussian effects. The method incorporates a parallel marginalization (PMMC) step in conjunction with the hybrid Monte Carlo (HMC) scheme to improve samples generated by standard particle filters. Parallel marginalization is an efficient Markov chain Monte Carlo (MCMC) strategy that uses lower dimensional approximate marginal distributions of the target distribution to accelerate equilibration. As a validation the algorithm is tested on a 2516 dimensional, bimodal, stochastic model motivated by the Kuroshio current that runs along the Japanese coast. The results of this test indicate that the method is an attractive alternative for problems that require the generality of a particle filter but have been inaccessible due to the limitations of standard particle filtering strategies.

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**MS78**

**Overview of Graduate CSE Education in Europe**

Nowadays CSE has been established as an academic discipline in the university and industry community. However, the interface to other disciplines is not so well defined which increases the variation of curricula of CSE programs to some extent. In this talk an overview of some European CSE programs will be presented with emphasis on development of curricula, the needs from academia and industry, and possible future scenarios of the education.

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**MS78**

**Report on International Study of Simulation-based Engineering & Science, and Preparing the Next Generation in CSE**

In this talk, we present an overview of the recent study "An International Study of Simulation Based Engineering and Science" sponsored by the National Science Foundation. We will focus on describing the state of CS&E graduate programs and training around the world. We will conclude with a description of a developing program "Virtual School of CSE".

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**MS78**

**CSE/CE Programs in Germany**

In recent years a remarkable variety of study programs in the field of Computational Science and Engineering emerged in Germany covering Bachelor, Master, and PhD education. A review on these developments will be provided. Similarities and differences in curricula, educational goals, and formal organization will be discussed. Conclusions on the success and the further development on these programs will be drawn.

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**MS78**

**CSE Graduate Programs in the US**

Abstract not available at time of publication.

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**MS79**

**Massively Parallel Ab Initio Electronic Structure and Molecular Dynamics Calculations**

First principle electronic structure and molecular dynamics calculations have evolved to become indispensable tools for the analysis and understanding of fundamendal properties of matter. These calculations have stretched our computational capabilities to their limits. Thus, their efficient deployment on massively parallel machines is absolutely crucial At the dawn of the petaflop era we will demonstrate that powerfull new numerical schemes in combination with well known workhorse kernels can achieve outstanding performance and results.

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**MS79**

**Algorithms for the Quantum Modeling the Properties of Nanocrystals, Nanofilms and Nanowires**

One of the most challenging issues in materials physics is to predict the properties of matter at the nanoscale. In this size regime, new structural and electronic properties exist that resemble neither the atomic, nor the solid state. By changing the size of the system, inherently intensive properties become extensive-like properties, which can be strongly altered from the macroscopic limit. Such properties can have profound technological implications, e.g., at small length scales a poor optical material like silicon can be converted to an optically active one.

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**MS79**

**Electronic Structure Calculations using FEAST**

A new robust and scalable algorithm, FEAST, for obtaining eigenvalues and eigenvectors of large sparse matrices will be presented. This algorithm deviates fundamentally from the traditional Krylov subspace based techniques (Arnoldi and Lanczos algorithms) or other

Davidson-Jacobi techniques, by exploiting general properties of density matrix in quantum mechanics. We will show how FEAST can take advantage of state-of-the-art system solvers either direct or iterative using quantum-based banded preconditioners, for performing large-scale ab-initio electronic structure calculations

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**MS79**

**Computational Challenges and Algorithms in Electronic Structure Calculations**

Density Functional Theory (DFT) is a successful technique used to determine the electronic structure of matter. It is derived from a number of approximations wich transform the original (intractable) Schrodinger equation to a nonlinear eigenvalue problem involving a set of one-electron eigenvectors. This problem is then solved iteratively with a so-called self-consistent field iteration. The challenge comes from the large number of eigenfunctions to be computed for realistic systems with, say, hundreds or thousands of electrons. We will discuss a parallel implementation of a finite difference approach for this problem and report on some results. We will also explore the fundamental underlying linear algebra which can be viewed as a problem of determining the diagonal of a projector associated with an invariant subspace. Methods that avoid completely the computation of eigenvectors will be briefly discussed. Finally, we will present some of the related challenging calculations such as one related to time-dependent density functional theory with an emphasis on showing some of the resulting big problems in matrix computation.

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**MS80**

**A Robust Mesh Untangling and Smoothing Method for ALE**

The rezone step in ALE methods relies on mesh smoothing that is perhaps triggered by mesh quality indicators to keep the computational mesh valid throughout a simulation. Most existing robust mesh untangling algorithms are minimization based and costly. In contrast, our 2D mesh untangling and smoothing algorithm is purely geometric, and as a result more efficient than minimization based approaches.

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**MS80**

**Mesh Optimization Based on Optimal Delaunay Triangulation**

In this talk, several mesh optimization schemes based on Optimal Delaunay triangulations (ODTs) are developed. Desirable meshes are obtained by minimizing the interpolation error in the weighted $L^1$ norm. Our schemes are divided into local and global two class. Several old and new local schemes, known as mesh smoothing, are derived from our approach. A graph Laplacian is used as a good preconditioner in the modified Newton method to speed up the traditional local smoothing approach. Our approach lay down the mathematical foundation on many mesh smoothing schemes used in practice and lead to a new global mesh optimization scheme. Numerical experiments indicate our method produce a well shaped triangulation in a fast way.

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**MS80**

**Mesh Adaptation by Monge-Kantorovich Optimization**

A new cell-area equidistribution method of grid adaptation, based on Monge-Kantorovich optimization, is presented [1, 2]. The method is based on a rigorous variational principle, in which the $L_2$ norm of the grid displacement is minimized, constrained locally to produce a prescribed positive-definite cell volume distribution. The procedure involves solving the Monge-Ampère equation: a single, nonlinear, elliptic scalar equation with no free parameters. Existence and uniqueness of solutions of the Monge-Ampère equation have been proved. For sufficiently small grid displacement, this method also minimizes the $L_2$ norm of the grid-cell distortion, measured by the trace of the metric tensor. We solve the Monge-Ampère equation numerically with a Jacobian-Free Newton-Krylov method. The ellipticity property of the Monge-Ampère equation allows multigrid preconditioning techniques to be used effectively, delivering a scalable algorithm under grid refinement. Several challenging test cases (in two and three dimensions and with complex domains) demonstrate the effectiveness of this method to produce optimal grids in which the constraint is satisfied numerically to truncation error. Furthermore, we show that the method is very robust against grid tangling and that, when compared to the well known deformation method [3], produces far better quality grids.

[1] G.L. Delzanno, L. Chacón, J.M. Finn, Y. Chung, and G. Lapenta, *An optimal robust equidistribution method for two-dimensional grid generation based on Monge-Kantorovich optimization*, to appear in *Journal of Computational Physics* (2008).

[2] J.M. Finn, G.L. Delzanno, and L. Chacón, *Grid generation and adaptation by Monge-Kantorovich optimization in two and three dimensions*, to appear in the *Proceedings of the 17th International Meshing Roundtable* (2008).

[3] G. Liao and D. Anderson, *A new approach to grid generation*, *Appl. Anal.* **44**, 285–297 (1992).

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**MS80**

**A Barrier-function Method for Mesh Quality Improvement**

We consider the problem of improving element quality in a finite element mesh by displacing its vertices. The problem of determining the optimal position of all vertices is a non-convex optimization problem. We write the objective function in a min-max form and then relax it with a log-barrier term to make it continuous. This constrained optimization problem is solved using an augmented Lagrangian method. Our results show quite successful mesh quality improvement.

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**MS81**

**Towards Full Braginskii Implicit Extended MHD**

Cold-ion extended MHD (XMHD) is an extremely challenging PDE system due to the presence of fast dispersive waves and of parabolic, anisotropic, parallel electron transport. Extending cold-ion XMHD to include warm-ion physics (such as finite-Larmor-radius (FLR) effects) adds to the challenge, as it supports additional dispersive (gyroviscous) waves. In this talk, we will dicuss progress in our fully implicit formulation towards including both parallel electron heat transport and ion FLR effects.

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**MS81**

**The Magnetic Reconnection Code: Using Code Generation Techniques in an Implicit Extended MHD Solver**

Abstract not available at time of publication.

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**MS81**

**Development and Applications of HiFi – Adaptive, Implicit, High Order Finite Element Code for General Multi-fluid Applications**

A three-dimensional (3D) implicit high order finite (spectral) element code HiFi, based on the well established two-dimensional SEL code[1], is now operational and continues to be developed at the PSI-Center of the University of Washington. The distinguishing capabilities of the code include fully 3D adaptive spectral element spatial representation with flexible multi-block geometry, highly parallelizable implicit time advance, and general flux-source form of the PDEs and boundary conditions that can be implemented in its framework. The two-dimensional version of the code has been extensively verified and used for simulations of various multi-fluid plasma physics phenomena, including magnetic reconnection, cylindrical tokamak sawtooth oscillations and FRC translation. The 3D code verification studies and the latest status of the code development effort will be discussed. This research is supported, in part, by the U.S. DOE Fusion Energy Postdoctoral Fellowship. [1] V.S. Lukin, Ph.D. Dissertation, Princeton University (2007).

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**MS81**

**Fully-Implicit Finite Element Formulations for Resistive Magneto-Hydrodynamic Systems**

In this presentation, we will discuss the development of multiple MHD formulations based on unstructured stabilized finite element methods including a 2D vector potential formulation and a 3D **B**-field formulation using projection. The resulting set of nonlinear equations is solved using fully-coupled Newton-Krylov solver. We will present numerical performance, accuracy, and initial scalability studies of the formulations. A stability and bifurcation analysis of the hydromagnetic Rayleigh-Bernard problem will be demonstrated.

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**MS82**

**Challenges of Scaling for Climate Dynamics**

Abstract not available at time of publication.

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**MS82**

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**MS82**

**A locally conservative spectral element dynamical core with non-oscillatory advection for the Community Climate System Model**

We present results from the integration of the highly scalable cubed-sphere atmospheric dynamical core HOMME into the Community Climate System Model (CCSM). CCSM/HOMME retains the excellent scalability of HOMME, running on 86,000 processors at a 25km average resolution. We use a new 4th order *compatible* formulation of the spectral element method, meaning it has discrete analogs of the key integral properties of the spherical div, grad and curl operators. This property allows the method to locally conserve both mass and energy. Compatibility also allows us to show that a purely element based reconstruction method is all that is needed to obtain monotone advection. With our initial reconstruction efforts, we obtain a 3'rd order accurate sign-preserving advection operator and a 2'nd order accurate monotone advection operator.

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**MS83**

**High Performance Systems Biology Simulation and Parameter Estimation: Addressing Uncertainties in Metabolic Models of** *Chlamydomonas reinhardti*

Modeling the entire metabolism in a biological organism demands the use of high-performance computer systems and the development of new software and computational approaches. In this talk, we discuss methodology and software tools we have developed for efficient simulation and parameter optimization of large-scale metabolic models. The approach we describe is the core of a parallel software package for solving problems that are beyond the scope of contemporary systems biology software. We concomitantly introduce and test the tools with a preliminary model of the primary and secondary carbon and hydrogen metabolism of the green alga *Chlamydomonas reinhardtii*.

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**MS83**

**Testing Alternative Models Using Cross Validation and Computationally Frugal Methods**

Many methods can be used to test alternative models. Tests considered here are for model discrimination (identifying models most likely to produce accurate predictions) and sensitivity analysis (identifying important observations and parameters). Computationally efficient model discrimination criteria and local sensitivity analysis and demanding cross-validation methods are compared using groundwater models of the Maggia Valley, Italy. Results show opportunities and difficulties of computationally frugal methods. This work is in collaboration with S.W. Mehl of the USGS and L. Foglia, P. Perona and P. Burlando of IfU, ETH Zurich.

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**MS83**

**A Geologically-Based Sequential Algorithm of Random Field Generation with Sparse Data**

Before running a porous media flow simulation, one must first characterize the types and locations of the soil comprising the subsurface region of interest. Hydrologists and Geologists use sparse data that is inherently uncertain to generate multiple realizations of the subsurface geometry as input to the porous media flow model. In this talk we discuss a new strategy for generating random fields using wellbore data and volume fraction estimates.

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**MS83**

**A Random-Field Based Orthogonal Expansion Method to Circumvent Curse-of-Dimensionality in Multiscale Modeling of Stochastic Systems**

The random variable based Polynomial Chaos (rv-PC) method, using Hermite and generalized PC, has been developed as a major numerical solver, which however can only tackle low dimensional problems with weak nonlinearity due to slow convergence of polynomial series and exponential increase of terms for non-Gaussian systems. In this talk we present a novel random field based orthogonal expansion (RF-OE) method to circumvent the curse-

of-dimensionality. The benchmark problems demonstrate a great computational advantage of the RF-OE method over the rv-PC method.

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**MS84**

**An Adjoint Study of Transient Decadal to Centenial Ocean Circulation Sensitivities**

We will present results from a study using the OpenAD open-source automatic differentiation tool. The OpenAD tool is applied to analyze the different sensitivities of poleward mass, heat and buoyancy transport in an ocean model (MITgcm) to boundary forcing. The sensitivities provide insight on possible broad-scale transient response of the ocean component of the climate system to changes in atmospheric and in lateral boundary fluxes.

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**MS84**

**Enhancing the Structural Index of Differential-algebraic Equations (DAEs) by Analysis of the Computational Graph**

The mathematical description of real-world problems, such as stemming from electrical engineering, often has a sparse computational graph. After disregarding this graph, this structure is not visible from the final equations. The computation of the structural index of DAEs a la Pryce is surprisingly simple, but fails in cases where the sparsity of the computational graph generates hidden functional dependencies. With the analysis of this graph we hope to somewhat remedy this problem.

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**MS84**

**Application of Automatic Differentiation with Code Coupling to Sensitivity and Uncertainty Analysis of Nuclear Systems**

The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) computational sequences within the SCALE code package utilize first-order perturbation theory to predict the response of neutron multiplication, $k_{\text{eff}}$, of a fissile system to changes in nuclear data values called cross sections. The TSUNAMI sequences calculate sensitivities implicit in the problem-dependent cross sections and propagate these sensitivities to the final $k_{\text{eff}}$ sensitivities. Automatic differentiation with code coupling was employed in these codes to produce the required sensitivity coefficients.

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**MS84**

**Automatic Differentiation via Source Transformation**

We will discuss the principles of implementing automatic differentiation (AD) with source transformation and where it is expected to be better than operator overloading. Using the OpenAD tool we will illustrate common usage patterns and highlight the major issues that impact the efficiency of the derivative computation. Taking an ocean model as an example we will explain how an AD tool can be integrated into models with a large and complicated source code base.

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**MS85**

**Optimal Experimental Design for Large Scale Nonlinear Inverse Problems**

Abstract not available at time of publication.

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**MS85**

**Model Reduction for Uncertainty Quantification in Large-scale Inverse Problems**

A reduced-order model is derived for the steady porous media flow equations with spatially-varying hydraulic conductivity. Parameter and state reduced bases are obtained simultaneously by iteratively sampling with a greedy approach. On each iteration, an optimization problem is solved to find the parameter field that maximizes the error between the high-fidelity and current reduced order model outputs. To solve the statistical inverse problem, we utilize the reduced-order model in a Markov chain Monte Carlo simulation. Realizations of the posterior probability density of the hydraulic conductivity field are used to compute a mean estimate and quantify uncertainty.

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**MS85**

**Bayesian Methods for Low Dose X-ray Tomogra-**

**phy**

X-ray tomography has become a routine diagnostic method in medicine, and there is a need to develop methods suitable for imaging with as low radiation dose as possible. The ALARA (As Low As Reasonably Achievable) principle in radiation protection states that low radiation exposure may be acceptable only if it cannot be avoided by reasonable procedures and if the task at hand cannot otherwise be completed. The radiation dose can be lowered by two different protocols, by lowering the X-ray source intensity or by diminishing number of projections used for the reconstruction. The former procedure means that at the limit, the signal becomes a photon count signal, while the latter one leads to the few radiograph tomography problem. Both approaches require new computational methods different from, e.g., the classical backprojection solution. In this talk, both of the dose lowering protocols are addressed and it is shown that using hierarchical Bayesian models, satisfactory fast reconstructions can be achieved.

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**MS85**

**Numerical Methods for Experimental Design of Large-scale Linear Ill-posed Inverse Problems**

While experimental design for well-posed inverse linear problems has been well studied, its ill-posed counterpart has received little attention. The ill-posed nature of the problem requires regularization techniques that introduce a bias that needs to be taken into account when choosing an experimental design. We discuss different ways to define an optimal design that controls both an average total error of regularized estimates and a measure of the total cost of the design. We also introduce a numerical framework that efficiently implements such designs and that can be used with large-scale problems. To illustrate the possible applications of the methodology, we consider a borehole tomography example and a two-dimensional function recovery problem.

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**MS86**

**Education Issues in CSE: Student Backgrounds, Instruction Modes, Outcomes**

One challenge in graduate CS&E education is dealing with diverse profiles of incoming students, with Bachelor degrees in engineering, natural sciences, computer science or mathematics. Depending on the desired graduate profile, a significant amount of curriculum flexibility may be necessary in order to harmonize the various skill sets. In addition, integrative instruction elements that combine various components of CS&E are called for, ranging from modifications to existing single-discipline courses to custom-designed laboratory modules and projects.

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**MS86**

**Ingredients of a CSE Education Program**

Abstract not available at time of publication.

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**MS86**

**Pros and Cons of CSE Programs Versus Disciplinary Programs, the Different Ways to Approach Training in CSE**

Abstract not available at time of publication.

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**MS86**

**SIAMs Role in Supporting and Developing CSE**

Abstract not available at time of publication.

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**MS87**

**Turbocharging Time Dependent Density Functional Theory with Lanczos Chain**

Using a super-operator formulation of linearized time-dependent density-functional theory, the dynamical polarizability of a system of interacting electrons is represented by an off-diagonal element of the resolvent of the Liouvillian superoperator, which can be efficiently evaluated using a newly devised Lanczos method. The resulting algorithm, which is particularly convenient when large basis sets are used, allows for the calculation of the full spectrum of a system with a computational workload of the same order as that needed for static polarizabilities within time-independent density-functional perturbation theory. The method is demonstrated with a few case molecular applications and compared with similar ideas used in other fields of science and engineering

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**MS87**

**A Linear Scaling Subspace Iteration Algorithm with Optimally Localized Non-Orthogonal Wave Functions for Kohn-Sham Density Functional Theory**

We present a new linear scaling algorithm, the Localized Subspace Iteration (LSI), for electronic structure analy-

sis using the Kohn-Sham density functional theory. This algorithm is based on subspace iteration and the non-orthogonal formulation of the Kohn-Sham functional, and it makes use of the improved localization properties of non-orthogonal wave functions. The efficiency and accuracy of this algorithm is demonstrated on fully three-dimensional analysis of the electronic structure of hydrocarbon chains.

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**MS87**

**Multipole Representation of the Fermi Operator and Linear Scaling Algorithm for Metallic Systems**

A new representation of the Fermi operator based on multipole expansion is introduced. The multipole representation is suitable for developing linear scaling algorithms for electronic structure calculation for both insulating and metallic systems.

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**MS87**

**Solving Nonlinear Eigenvalue Problems in Electronic Structure Calculations**

One of the key tasks in electronic structure calculation is to solve a nonlinear eigenvalue in which the matrix Hamiltonian depends on the eigenvectors to be computed. This problem can be solved either as a system of nonlinear equations or as a constrained nonlinear optimization problem. We will examine the numerical algorithms used in both approaches and compare their convergence properties. We will also discuss the use of Broyden updates and trust region techniques in these algorithms.

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**MS88**

**Variational Methods for Hexahedral Mesh Quality Improvement**

In this talk I shall briefly survey the approach of variational methods in quadrilateral/hexahedral mesh quality improvement. I shall then contrast the choice of a few different high-order energy functionals by their Euler-Lagrange equation i.e a non-linear elliptic or biharmonic partial differential equation (PDE), and the discretization formulas of the differential operators. Finally, I shall describe several applications of these methods in producing feature preserving, quality quadrilateral / hexahedral meshes.

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**MS88**

**Optimal and Quasi-optimal Meshes for Minimizing the Interpolation Error and its Gradient**

We present and analyze a new technology for generating meshes minimizing the interpolation error or its gradient. The key element of the methodology is the construction of a metric from node-based and edge-based values of a given function. For a mesh with $N$ triangles, we prove that the interpolation error is proportional to $1/N$ and the gradient error is proportional to $1/\sqrt{N}$ which are the optimal asymptotics. The methodology can be applied to adaptive solution of PDEs provided that edge-based a posteriori error estimates are available.

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**MS88**

**Improving the Hexahedral Quality Obtained From Streaming Mesh Refinement**

Geometric quality results are presented for an embarrassingly parallel method to refine unstructured convex hexahedral meshes. The method decomposes an input hexahedron into smaller hexahedra given the pattern of division of its twelve edges, each either left intact or divided in three. While the common faces of adjacent hexahedra must match automatically without communication, some freedom in decomposition templates and vertex placement can be used to improve the quality of the refined mesh.

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**MS88**

**Title not available at time of publication**

In general, the higher the quality of the elements of a mesh the better it is for solving an application problem modeled by this mesh. A number of algorithms and software has been developed over the last two decades for computing graded meshes with guaranteed quality. However, these methods tend to fail catastrophically when the mesh elements are expected to be very high quality (e.g., all angles larger than 40 degrees and/or all angles strictly less than 90 degrees). We present new algorithms and software for computing premium quality graded meshes.

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**MS89**

**Level Set Simulation of Coupled Advection-diffusion and Pore Structure Evolution due to Mineral Precipitation in Fractured and Porous Media**

The coupled processes of fluid flow, solute transport and mineral precipitation/dissolution in porous media are of great interest in a large variety of scientific and engineering areas. A pore-scale simulation technique, based on level set interface tracking, was developed for modeling such coupled processes and reaction induced pore geometry evolutions, under various of transport and reaction regimes. Quantitative relationships between permeability and porosity were obtained and discussed.

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**MS89**

**Fast and Accurate Numerical Approaches for Stefan Problems and Crystal Growth**

New numerical approaches for moving boundary/interface applications tailored for Stefan problems and crystal growth simulation are discussed in this talk. The focus is placed on the issues of accuracy and speed-up. A modified Crank-Nicolson method which is second order accurate and stable is developed. The ADI (alternating directional implicit) method is also developed to speed up the simulation for a certain class of problems. The ADI method is shown to be asymptotically stable and at least first order accurate. Numerical results, however, show that the ADI method actually provides second order accuracy if the velocity can be calculated accurately. The level set method is used to update the moving interface so that the topological changes can be handled easily. Numerical experiments are compared to exact solutions and those results in the literature.

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**MS89**

**Application of Front Tracking to Crystal Growth with Large Damkohler Number**

Crystal growth is a phase transition problem with a dendritically advancing front. The interface velocity is a local function and the fractal structure requires high interface resolution. This makes the Lagrangian front tracking an ideal method. Our numerical simulation using the FronTier code showed very good agreement with the SPH method on fractal dimension and average growth rate. We will also analyze the curvature effect on the simulation with high Damkohler number.

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**MS89**

**Phase-Field Model for Crystal Growth in a Bridgman Furnace**

A phase-field based model was developed to study the crystal growth in Bridgman systems. The model takes into account effects of melt convection, anisotropy in kinetic and interfacial free energy coefficients as well as the effect of the front curvature on the crystal growth. The model was used to study the effect of the orientation of preferred crystal growth directions with respect to the longitudinal axis of the furnace.

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**MS90**

**Convergence of Spectral Polynomial Chaos Approximation for SPDES**

We will discuss the convergence of spectral polynomial chaos approximations for stochastic elliptic equations with random diffusion coefficients. We will consider two different settings: Wick product and regular product. In the Wick product case, we are able to derive the rate of convergence. In the regular product case, we are able derive the convergence result.

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**MS90**

**Stochastic Analysis of a Nanoresonator with Random Geometry**

We present the application of the polynomial chaos

methodology to the analysis of a nanoresonator exhibiting random geometry. The physical problem involves strong interactions between mechanical and electrostatic fields which are exaggerated due to the effects of random shape. We describe the nominal problem using a deterministic shape to which the random shape is referenced via a nonlinear transformation the jacobian of which is described in terms of its polynomial chaos decomposition. We demonstrate efficiency and robustness of the proposed methodologies.

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**MS90**

**Uncertainty Quantification in Chemical Systems**

This talk will demonstrate the use of multiwavelet spectral polynomial chaos (PC) techniques for uncertainty quantification in ignition of a methane-air system at atmospheric pressure. Bayesian inference is employed for identifying the probabilistic representation of the uncertain parameters based on data. These random/uncertain parameters are represented using multiwavelet PC, and the uncertainty is propagated through the ignition process using both intrusive Galerkin projection and non-intrusive monte-carlo sampling methods. We analyze the time evolution of moments and probability density functions of the solution, and examine the role and significance of dependence among the uncertain parameters. We finish with a discussion of the role of nonlinearity and the performance of the algorithm.

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**MS90**

**Uncertainty Quantification for Elliptic Equations of Arbitrary Stochastic Order**

Uncertainty quantification for elliptic PDEs with random coefficients will be discussed. A typical example of interest is the following model described by the Dirichlet problem:

$$-\sum_{i,j=1}^{d}\left(a_{ij}\left(x,\omega\right)u_{x_i}\left(x,\omega\right)\right)_{x_j}=f\left(x\right),x\in\mathcal{O},\sqcap_{|\partial\mathcal{O}}=\}\left(\S\right), \tag{1}$$

It will be assumed that $a\left(x,\omega\right)=a\left(x,\bar{\xi}\right)$ where $\bar{\xi}$ is a sequence of independent Gaussian $(N(0,1)$ random variables. This model has been studied extensively in the uncertainty quantification literature. Two types of assumptions were normally considered:

$$a(x,\omega)=\bar{a}(x)+\epsilon(x,\bar{\xi})$$

or

$$a(x,\omega)=c\exp\left\{\bar{a}(x)+\epsilon(x,\bar{\xi})\right\},$$

where $\bar{a}$ is the mean and the noise $\epsilon=\sum_{i=1}^{\infty}\sqrt{\lambda_i}h_i(x)\xi_i$. The first model is stochastically linear in that its Wiener chaos expansion contains only zero and first order Hermite polynomials. In the second case the stochastic order is infinity. Well-posedness problem of (1) for $a(x,\bar{\xi})$ of any stochastic order as well as related numerical approximations and truncation errors will be discussed.

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**MS91**

**Nonlinear Multigrid Methods for Fully Implicit Resistive MHD Simulations**

Nonlinear multigrid algorithms are discussed in the context of fully implicit resistive MHD simulations. F-cycle multigrid methods, in theory, reduce the algebraic error in nonlinear equations to the order of the discretization error in one iteration, thereby allowing for minimal work per time step (equivalent to about 7 residual calculations) in a fully implicit time integration simulation. We investigate the application of these nonlinear multigrid methods on some common benchmark 2D problems in resistive MHD.

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**MS91**

**Implicit Adaptive Mesh Refinement for 2D Resistive Magnetohydrodynamics**

Application of implicit adaptive mesh refinement (AMR)

to a 2D reduced resistive magnetohydrodynamics (MHD) model is described. This challenging, multi-scale, multi-physics model is of interest for the understanding of magnetically-confined plasmas. AMR is employed to resolve extremely thin current sheets, essential for an accurate macroscopic description. Implicit time stepping allows us to accurately follow the dynamical time scale of the developing magnetic field, without being restricted by fast Alfven time scales. At each time step, the large-scale system of nonlinear equations is solved by a Jacobian-free Newton-Krylov method together with a physics-based preconditioner. Each block within the preconditioner is solved optimally using the Fast Adaptive Composite grid method, which can be considered as a multiplicative Schwarz method on AMR grids. In this talk, we will discuss the application of the algorithm to several challenging MHD applications. It will be demonstrated that the approach behaves optimally (scalably) under grid refinement, and that numerical error in the solution is independent of the number of refinement levels. Furthermore, for the applications explored, the AMR approach results in substantial CPU savings (more than 80%) vs. what would be required by an equivalent uniform-mesh simulation.

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**MS91**

**A Preconditioned JFNK Method for Resistive MHD in a Mapped-grid Tokamak Geometry**

We present a fully-implicit Newton-Krylov method for MHD simulations in a tokamak employing a curvilinear grid in the poloidal cross-section. The operator-based preconditioning of the stiff hyperbolic components comprises of directional splitting followed by a characteristic decomposition of the directional parts. This method allows us to precondition all the ideal-MHD waves or only the stiffest ones (e.g. only the fast compressive wave in the poloidal planes). We demonstrate our method by fusion MHD examples. Supported by USDOE Contract no. DE-AC020-76-CH03073 and USDOE SciDAC Contract ER25785.

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**MS91**

**Progress in Parallel Implicit Methods for Tokamak Edge Plasma Modeling**

Performance of prototype tokamak fusion devices depends sensitively on characteristics of the edge plasma between the hot core and surrounding walls. This presentation introduces some of the benefits and challenges of parallel implicit solution strategies, which have proven to be effective in handling these challenges in tokamak edge plasma modeling. We discuss experience with preconditioned Newton-Krylov methods in parallel edge plasma transport, with emphasis on scalable algorithms and implementations in the BOUT and UEDGE applications.

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**MS93**

**A Free Boundary Problem with a Moving Contact Line**

The motion of a drop on a solid surface has been a subject of extensive research. The model is the Navier Stokes equations for the fluid, and the Navier boundary condition at the contact line between the fluid and the solid. Often the model is a two-phase flow with a moving contact line and triple junctions. Under some circumstances, the one-phase model may be appropriate so that the problem can be solved more efficiently. In this talk, I will first introduce the model, and then introduce the augmented immersed interface method for the problem. In this approach, we introduce augmented variables so that (1), we can get an efficient discretization; (2) fast solvers on regular domains can be utilized. This new augmented immersed interface method has been applied to a number of problems for Stokes and Navier Stokes flows, problems on irregular domains. Numerical example will also be presented.

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**MS93**

**Instabilities, Pattern Formation and Mixing in Active Particle Suspensions**

A kinetic theory is developed and applied to study the complex dynamics and pattern formation arising in suspensions of hydrodynamically interacting self-propelled particles, such as swimming microorganisms. The stability of isotropic suspensions is first investigated, and we demonstrate the existence of an instability in which shear stresses are eigenmodes. Nonlinear effects are also studied using numerical simulations in two dimensions, and are shown to be characterized by strong density fluctuations and very

efficient fluid mixing.

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**MS93**

**Direct Simulation of Anatomical Flows using Embedded Boundary Methods**

We use the embedded boundary method to discretize flow equations in real anatomies. Flow geometries are obtained without loss in geometric detail from level set techniques applied to patient-specific image data. A higher-order volume-of-fluid approach is taken in irregular Cartesian grid cells that are cut by the embedded boundary domain; standard finite difference discretizations are applied away from the boundary. We present resolved 3D simulation results of flows in a carotid artery and a trachea.

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**MS94**

**A Kinematically Coupled Scheme for Fluid-structure Interaction in Blood Flow**

In this work we present the latest application to fluid structure interaction in arterial blood flow of a newel operator splitting technique. Partitioned algorithms are based on the idea of splitting the full problem in simpler subproblems which summed give the original full problem. The coupling at the interface between blood and arterial wall is highly nonlinear because the ratio between fluid and structure density is closed to one; this is the reason why many partitioned schemes successfully applied in aeroelasticity fail when applied to blood flow simulations. Our partitioned scheme, based on a time discretization via operator splitting, uses the kinematic condition at the interface to couple fluid and structure velocities at each sub-step and here is presented to successfully describe arterial wall motion and blood flow

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**MS94**

**Modeling, Analysis and Simulation in Blood Flow**

Modeling blood flow in compliant vessels presents very challenging tasks from both the analytical and computational points of view. In this talk, we will present recent advances in both the theoretical and the numerical aspect of blood flow modeling in compliant vessels and we will show how these two aspects are tightly related.

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**MS94**

**Numerical Model Adaptivity and Domain Decomposition in Electrocardiology**

Action potential propagation in the myocardial tissue is described using the Bidomain macroscopic model, coupled with models for the ionic cell currents (Rogers-McCulloch, Luo-Rudy). Since solving the Bidomain model is very expensive, methods to reduce its computational costs without losing accuracy are investigated. In particular we present a model adapting strategy based on the simplified Monodomain model and coupled with domain decomposition techniques.

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**MS94**

**Dissipative Effect of Chaotic Boundary Motion on an Incompressible Viscous Flow**

We consider the NavierStokes equations with quasi-periodic and chaotic moving boundary. Numerical experiments are specially designed to keep the volume of the domain constant at all times. We compare the averaged properties (e.g. flux) of the flow with the Poiseuille profile for the fixed domain of the same volume. Dependence of the averaged flux on the magnitude and frequency of the boundary motion is considered in detail.

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**MS95**

**Bayesian Inference of Biochemical Reaction Networks**

Biochemical reaction models of cell signaling pathways greatly aid to analyze the function and control of processes such as the human immune response. However, inferring robust and accurate signaling models from experimental data is challenging as measurements are noisy, limited to few proteins, at sparse instances in time, from heterogeneous sources. We present the development of Bayesian methods for model inference and comparison applied to cell signaling pathways in the human innate immune response.

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**MS95**

**No-think MCMC Sampling for EIT and Other Inverse Problems**

Newcomers to computational inference for inverse problems face the (steep) learning curve of building and tuning proposals for MCMC sampling algorithms if they want reasonable convergence times. This is because representations usually live in high-dimensional spaces, and the ill posedness causes posterior distributions to have correlation coefficients of 1-0. The t-walk is a general purpose, black box, sampler that can adequately sample many of these problems, and lets scientists get on with other jobs.

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**MS95**

**A Sparse Grid Collocation Approach to Solving Stochastic Inverse Problems**

A scalable, parallel methodology for stochastic inverse/design problems is presented. The representation of the underlying uncertainties and the resultant stochastic dependant variables is performed using a sparse grid collocation methodology. The stochastic inverse/design problem is transformed to a deterministic optimization problem in a larger-dimensional space that is subsequently solved using deterministic optimization algorithms. The design framework relies entirely on deterministic direct and sensitivity analysis of the continuum systems. Gradient based and Gradient free optimization strategies are utilized and their performance compared. Various illustrative examples with multiple sources of uncertainty are provided to showcase the developed framework.

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**MS95**

**Variance Reduction for Particle Filters of Systems with Time-scale Separation**

We present a particle filter construction for a system that exhibits time-scale separation. This allows two simplifications: i) The use of the averaging principle for the dimensional reduction of the system needed to solve for each particle and ii) the factorization of the transition probability which allows the Rao-Blackwellization of the filtering step. The resulting particle filter is faster and has smaller variance than the particle filter based on the original system.

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**MS96**

**Sparse Tensor Discretization of Elliptic sPDEs**

We present a novel class of sparse tensor discretizations for the numerical solution of elliptic sPDEs. It is based on a separated, parametric representation of the input random fields such as a Karhunen-Loeve expansion, and a Galerkin type projection of the unknown, parametrized random field solution onto 'polynomial chaos' type, spectral discretizations. Implementation demonstrates robustness of the method even for input data with small spatial correlation length, i.e., for a slowly converging Karhunen-Loeve expansion of the random field inputs.

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**MS96**

**High Order Stochastic Simulations for Problems with Discontinuous Random Space**

The general need for effective uncertainty quantification in engineering problems has been a catalyst for the development of stochastic computational modeling. When a deterministic model, described by a system of partial differential equations (PDEs), is used to generate a stochastic model, or system of stochastic partial differential equations (SPDEs), the space associated with the SPDEs grows to include the original space/time dimensions of the PDEs and additional random dimensions determined by the nature of the random inputs. Preserving accuracy and minimizing computational cost requires the utilization of higher order methods, such as generalized polynomial chaos (gPC). Typical of higher order methods, gPC has fast convergence properties when solutions are sufficiently smooth. However, when discontinuities arise in the solutions of SPDEs, the convergence rate of gPC suffers. This talk will demonstrate how the incorporation of multi-dimensional discontinuity detection can be joined with gPC to provide computationally efficient, high order approximations to SPDEs that contain discontinuities in the solution and/or random space.

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**MS96**

**Uncertainty Quantification for Flow and Transport in Randomly Heterogeneous Porous Media**

Porous media in nature is highly heterogeneous and subject to uncertain due to the lack of sufficient data. Multiscale of uncertainty is present between and within the layers of porous media. A general framework that combines random domain decompositions (RDD) and probabilistic collocation method on sparse grids is proposed to resolve the large- and small-scales of uncertainty effectively. This combined approach is applied to investigate the flow in subsurface randomly heterogeneous porous media and the nuclear contaminants transport in DOE Hanford site.

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**MS96**

**Numerical Strategy for Problems with Random Geometry**

While many determinisitc and stochastic simulations assume computational domain is known precisely and with fixed geometrical definition. In practice, however, the domain can be a major source of uncertainty in many applications because it can not be determined precisely. In this talk we discuss various available techniques, such as random mapping, domain perturbation, etc., to recast the problems in uncertain geometry to ones in fixed geometry, which then allow applications of standard numerical analysis. As an example, we discuss an efficient numerical algorithm for acoustic scattering problem over a rough object.

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**MS97**

**The FETI Family of Domain Decomposition Methods for Inequality Constrained Quadratic Programming: Application to Contact Problems**

Two domain decomposition methods for solving iteratively quadratic programming problems with linear inequality constraints are presented. These methods are based on the FETI and FETI-DP algorithms, and solve an equivalent constrained problem by an active set strategy and a nonlinear conjugate gradient method equipped with controls to guarantee convergence monotonicity. Their scalability is illustrated on a Linux cluster for a complex 1.4 million degree of freedom multibody problem with frictionless contact and nonconforming discrete interfaces.

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**MS97**

**Direction-preserving and Schur-monotonic Semiseparable Approximations of Symmetric Positive Definite Matrices**

For a given symmetric positive definite matrix $A \in \mathbf{R}^{n\times n}$, we develop a fast and backward stable algorithm to approximate $A$ by a symmetric positive-definite semi-separable matrix, accurate to any prescribed tolerance. In addition, this algorithm preserves the product, $AZ$, for a given matrix $Z \in \mathbf{R}^{n\times d}$, where $d \ll n$. Our algorithm guarantees the positive-definiteness of the semi-separable matrix by embedding an approximation strategy inside a Cholesky factorization procedure to ensure that the Schur complements all remain positive definite after approximation. We present numerical results and discuss its potential of being used as a fast solver for dense and sparse linear systems.

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**MS97**

**Parallel Preconditioning of Linear Systems based on ILUPACK for Multithreaded Architectures**

We investigate the efficient iterative solution of large scale sparse linear systems on shared-memory multiprocessors. In particular, our parallel approach is based on a multilevel ILU preconditioner which preserves the mathematical semantics of the sequential method in ILUPACK. Here we exploit the parallelism exposed by the task tree associated with the problem (task parallelism), employ dynamic scheduling of tasks to processors to improve load balance, and formulate all stages of the parallel PCG method conformal with the computation of the preconditioner to increase data reuse. Results on a CC-NUMA platform with 16 processors reveal the parallel efficiency of this solution.

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**MS97**

**Preconditioning Techniques for a Hybrid Method to Solve Highly-Indefinite Linear Systems**

In many modern scientific simulations, solving linear systems of equations is a bottleneck. These linear systems are often so large that direct methods would require infeasibly-large amounts of memory. At the same time, these systems are highly-indefinite, and preconditioned iterative methods suffer from slow convergence. In this talk, we present a hybrid method and effective preconditioning techniques to solve this type of linear system.

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**MS98**

**Use of High-Level User Interfaces for Software Sustainability**

Here we discuss a high-level user interface to the DOE Advanced CompuTational Software (ACTS) Collection, PyACTS. PyACTS speeds-up the software development cycle by assisting the user with a first coding solution using tool in the ACTS collection. The interface is also used for expressing tool dependencies and automatic testing and validation. The latter is part of larger infrastructure within the ACTS project that support software sustainability.

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**MS98**

**FiPy: A PDE Solver for Materials Science**

Many existing PDE solver packages focus on the important, but arcane, task of actually numerically solving the linearized set of algebraic equations that result from the discretization of a set of PDEs. The need for many researchers is higher-level than that. This talk presents FiPy, a Python-based environment for easy specification of PDE problems. Examples on applications to research problems in material science are provided.

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**MS98**

**A Python-Based Persistence and Software Component Framework for Scientific Computing**

We address the issues surrounding checkpointing, restart, precompile/precompute and staging of scientific codes. Systematic handling of these issues in a C/C++ framework is tedious and requires an interaction with the operating system, leading to poor portability. Therefore, it appears natural to implement a relatively high-level component and persistence framework in Python. We demonstrate the framework in molecular dynamics and finite element simulations.

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**MS98**

**Experience with Python in a Major Computational Science Teaching Reform**

Numerical programming and simulation are now becoming key tools in a wide range of science courses the University of Oslo. Python is chosen as the dominating platform for this reform. We discuss the background for this choice and the

experience with using Python, we describe an introductory scientific programming course based on Python, we present various Python tools for handling graphics and simulation, and we discuss how Python combines with Matlab, Fortran, C and C++.

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**MS99**

**Multi-Physics Modeling of High Explosives**

High explosives (HE) applications are often characterized by multi-scale and multi-physics phenomena. Detonation waves, a coupling between chemistry and compressible flow, are characterized by length scales that are hundreds or thousands of times smaller than the eventual devices of interest. Furthermore It is often important to include coupling effects between the HE and an inert material. This talk investigates computational aspects of these multi-physics effects focusing in particular on the coupling to inert materials.

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**MS99**

**Coupled Simulation of Thin Solid Structures Subjected to Shock Waves in Liquids**

The construction of efficient and scalable algorithms for simulating shock-driven fluid-structure interaction problems is a challenging task. We have devised a generic coupling approach that combines Cartesian dynamically adaptive shock-capturing methods with solid mechanics solvers for elasticity, visco-plasticity, and fracture. The focus of this presentation lies on reproducible verification and validation configurations for shock impact on thin circular structures in liquids and the additional challenges, compared to gas dynamics, that had to be overcome.

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**MS99**

**A Composite Grid Solver for Conjugate Heat Transfer Problems**

We describe a numerical method that uses overlapping grids for simulating conjugate heat transfer problems that involve incompressible fluid flows coupled to heat conduction in solids. The computational region is divided into a number of sub-domains corresponding to fluid domains and solid domains. Different physics solvers are associated with each domain. The solution is advanced in a weakly-coupled fashion. We discuss different approximations to the interface conditions and different algorithms for solving the coupled problem.

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**MS99**

**Multiphysics Computations for Models of Reactive Flow**

The aim of this talk is to describe recent and ongoing research into multiphase models of condensed-phase, high-energy explosives. These materials have a complex microstructure in which the grains of the explosive component are held together by an inert plastic binder, and voids and pores abound within the granular aggregate. Mathematical models of these materials involve equations for both solid and fluid mechanics. The talk will focus on our recent efforts to develop numerical methods for this multi-physics application within a structured overlapping grid framework with adaptive mesh refinement. Results for one and two-dimensional reactive flow problems will be presented.

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**MS101**

**Hybrid Parallelism in Scientific and Engineering Applications First Steps**

Application scalability on HPC systems with multicore processing nodes requires hybrid (inter/intra-node) parallelism. Data-parallelism via MPI has become the defacto-standard for inter-node parallelism. Given the diversity of multicore nodes, each with its peculiar memory architecture and interface, an intra-node standard is unlikely in the near term. We are investigating how to restructure applications and libraries to (1) enable decoupled inter/intra-node parallelism and (2) sufficiently isolate intra-node parallelism to ease future porting to varied multicore architectures.

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**MS101**

**Software Design Issues for Scalable Multicore Computers**

The advent of multicore processors presents a tremendous opportunity and challenge to CSE applications and libraries developers. On the one hand we have the opportunity to achieve an order of magnitude or more performance improvement if we can harness multicore capabilities, on the other we are presented with a significant algorithm and software redesign in order to realize this improvement. In this presentation we discuss performance characteristics of current multicore processors and provide a brief assessment of current multicore programming models. We finally discuss plans in the Trilinos project to develop portable ca-

pabilities for scalable multicore computers.

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**MS101**
**Tree-based Methods on GPUs**

We examine the performance of the Fast Multipole Method on the Nvidia Tesla machine. The inherent bottleneck imposed by the tree structure is ameliorated by a refactoring of the algorithm which exposes the fine-grained dependency structure. Examples are shown for problems arising from vortex methods for fluids.

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**MS101**
**Multicore Processing in ANSYS Simulations: Problems, Progress and Promise**

Multicore processing has potentially changed the landscape of software simulation capabilities offering an affordable computing environment where the number of computers available for simulation far exceeds the number of analysts using the resource. In spite of this potential the current environment has only begun to tap the potential of multicore processors. This talk will focus on some of the challenges in using multicore processors in compute and I/O intensive simulation software. The challenges include balancing multicore CPUs with limited memory bandwidth and shared I/O resources and harnessing the potential of various CPU accelerator devices. An overview of shared memory and distributed memory parallel processing in ANSYS will be given along with some results from recent progress with GPU acceleration of solvers. Finally, the promise of multicore processing in advancing simulation software capabilities in industry will be discussed.

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**MS102**
**Sharing Computational Science Instructional Materials through a Peer Reviewed Process**

This session presents the newly launched Journal of Computational Science Education. The journal focuses on computational science lesson plans, exercises, programs, datasets, and technical papers describing the outcomes of computational science education. The peer review process provides an incentive for people to submit items to the journal and also assures those that use the materials that they have been validated, verified, and accredited for use in the educational settings for which they were intended.

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**MS102**
**Petascale Computing Education**

Abstract not available at time of publication.

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**MS102**
**Spreading the Word with Spread-of-Disease Modeling**

Disease transmission models have helped form successful strategies for managing epidemics, but science students are usually unaware of their advantages and challenges. Thus, we designed laboratories on the modeling of the spread of disease for introductory microbiology. Students in Wofford's Emphasis in Computational Science, who study modeling and simulation in depth, were assistants for the sequence of three laboratories. The sequence improved student understanding of human disease dynamics and demonstrated the utility of mathematical models.

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**MS102**
**SIURO: SIAM Undergraduate Research Online**

The value of research experiences for students, and its use in recruiting good students are well understood and form a background to this talk. SIURO provides an excellent outlet for publishing students research results. This new publication has recently been launched by SIAM. The inaugural EIC will describe the publication and its role. SIURO provides an excellent outlet for undergraduate research and provides a resource for identifying potential graduate students or research assistants for faculty.

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**MS103**
**Investigations of Biomorphic Aquatic and Aerial Locomotion with the Dynamically-coupled Viscous Vortex Particle Method**

Biomechanics of moderate Reynolds number locomotion are characterized by the reaction force supplied by the fluid against deforming structures and the vortical wake produced by this interaction. Motivated by such problems, we present the development of a viscous vortex particle method with coupled body dynamics. The previously developed and validated tool for two-dimensional problems is briefly reviewed. The method is extended to three-dimensional problems, and the various components of the

solver are highlighted.

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**MS103**

**An Integrative CFD Model of Lamprey Swimming**

Swimming due to sinusoidal body undulations is observed across the full spectrum of swimming organisms, from microscopic flagella to fish. These undulations are achieved due to internal force-generating mechanisms, which, in the case of lamprey are due to a wave of neural activation from head to tail which gives rise to a wave of muscle activation. Here we present recent results on a computational model of a swimming lamprey that couples activation of discrete muscle segments, passive elastic forces, and a surrounding viscous, incompressible fluid. The fluid dynamics is modeled by the Navier-Stokes equations at appropriate Reynolds numbers, where the resulting flow field and vortex shedding may be measured.

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**MS103**

**Fish Locomotion: Multiple Wake Interactions**

This research investigates the behavior of an infinite array of (inverse) von Karman streets. While the dynamics and stability of a single vortex street is well-understood, little work is done on the interaction of multiple streets. Our primary motivation is to model the wake dynamics in large fish schools. We ignore the fish and focus on the dynamic interaction of multiple wakes where each wake is modeled as an inverse von Karman street. In particular, we investigate the problem of fluid transport between adjacent streets for its relevance to understanding the transport of oxygen and nutrients to inner fish in large schools as well as understanding flow barriers to passive locomotion.

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**MS103**

**Integral Theorems for Locomotion in Complex Fluids**

Many problems in cell locomotion involve the swimming of organisms in non-Newtonian fluids (e.g. spermatozoa in cervical mucus). In this work, we present quantitative models of cell locomotion in polymeric solutions. We first derive integral equations which allow to calculate directly the swimming kinematics for a cell moving in a polymeric solution by using only the solution of the Newtonian swimming problem. We then illustrate how these results can be applied to real biological swimmers.

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**MS104**

**A Dynamic Programming Approach to Auto-Tuning the Blocking Strategy For the Householder QR Decomposition**

Blocking techniques are widely used for high performance computation of the Householder QR decomposition. However, the optimal blocking strategy differs depending on the target architecture and the problem size. In this study, we present a new approach to auto-tuning the blocking strategy. We parameterize blocking strategies and find the near-optimal one using dynamic programming. Experimental results show that our approach can achieve the same level of performance as that obtained by manual tuning.

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**MS104**

**Impact of Auto-tuning for a Sparse Iterative Solver on a Multicore Windows Cluster**

An automatic performance tuning is a key component of getting high performance for a variety of problems. This is important even when a platform is changed or upgraded. Therefore, we need to consider many system configurations. First, the auto-tuning methodology of our solver is presented. Then, the effect of auto-tuning and the performance on a multicore Windows cluster is introduced.

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**MS104**

**An Experiment of Tall Skinny type QR-factorization on a Multicore CPU System and a Small SMP System**

An experiment of the Tall Skinny type $QR$-factorization is made on a multicore CPU system and a small SMP multi-

core CPU system.

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**MS104**

**A Volumetric 3-D FFT on Clusters of Multi-Core Processors**

In this talk, a volumetric three-dimensional fast Fourier transform (FFT) algorithm on clusters of multi-core processors is presented. An efficient data distribution for three-dimensional FFT is given with confirmation of the theoretical analysis. Performance results of volumetric three-dimensional FFTs on clusters of multi-core processors are reported.

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**MS105**

**A Parallel Mesh Interface for Interoperable Mesh-based Tools**

We describe ITAPS' parallel mesh interface and its use in interoperable mesh-based tools. The parallel mesh interface accesses meshes distributed over parallel computers, and supports services such as parallel mesh adaptivity, mesh quality improvement, and dynamic load balancing. The parallel interface supports the basic data model of ITAPS' serial mesh interface while adding a partition model of mesh distributions. We describe this partition model and the parallel interface, and present examples using interoperable mesh services.

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**MS105**

**An Overview of ITAPS Interoperable Mesh and Geometry Technologies**

Interoperable mesh and geometry technologies developed by the ITAPS center allow domain scientists to leverage both software and the expertise of tool developers. In this talk I provide an overview of the ITAPS efforts, particularly focusing on the technologies required to create interoperable software; namely a set of common interfaces that balance performance and flexibility, the tools used to address language interoperability issues. I introduce the many tools that are available to application scientists through the ITAPS interfaces and show examples of their use in SciDAC applications.

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**MS105**

**A Finite-Volume Method for Anisotropic Hybrid Mesh Adaptivity**

We present in this research the development of a coupled rh-hybrid adaptive meshing method tailored to applications in multi-physics simulation. This method proposes an adaptation method based on the combination of both element subdivision (h-adaptivity) and node point repositioning (r-adaptivity). By combining the two methods using the notion of a "mobility function", the proposed approach seeks to increase the flexibility and extensibility of mesh motion algorithms while providing a smoother transition between refined regions. The constrained adaptive method helps in limiting the size of the mesh than is produced by element subdivision alone. The method employs a rigorous constrained minimization approach, and results in a single elliptic nonlinear PDE system derived from anisotropic quasiconfomal mapping. An unstructured cell-centered finite-volume approach is used for solving the adaptive elliptic system for general polygonal meshes.

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**MS105**

**Supporting Parallel Adaptive Simulations through the iMeshP Interface**

The ability to support adaptive unstructured mesh simulations over complex geometries requires general mesh adaptation tools that are able to perform general mesh refinement and coarsening including the creation of anisotropic meshes and accounting for curved geometries. This talk will discuss progress to date on using the iMeshP interface to couple a general parallel mesh adaptation procedure with parallel unstructured mesh solvers to create fully par-

allel adaptive simulation procedures.

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**MS106**

**An Implementation of the Iterative Rational Krylov Method for Optimal H2 Model Reduction**

The IRK method has recently attracted attention because of its effectiveness in real world applications, as well as because of its mathematical elegance. We analyze the convergence of fixed point iterations behind the IRK idea, and show how proper stopping criterion translates into a backward stability relation. Both issues (convergence, stopping criterion) have impact on the floating point implementation. We will present a new mathematical software, based on the new theoretical development.

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**MS106**

**An Interpolation-Based Approach to Optimal $H_\infty$ Model Reduction**

We propose an interpolation-based approach to optimal $H_\infty$ model reduction. The proposed method constructs an optimal $H_2$ approximation using the IRKA method of Gugercin, Antoulas and Beattie and then solves a minimax problem to alter this approximation with the D-term that minimizes the $H_\infty$ norm of the error-system. We focus on state-space symmetric systems and discuss the extension to the general non-symmetric case. Several examples show that the approach consistently outperforms balanced truncation.

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**MS106**

**H2-optimal Approximation of MIMO Linear Dynamical Systems**

We consider the problem of approximating a multiple-input multiple-output (MIMO) $p \times m$ rational transfer function $H(s)$ of high degree by another $p \times m$ rational transfer function $\hat{H}(s)$ of much smaller degree, so that the $\mathcal{H}_2$ norm of the approximation error is minimized. We characterize the stationary points of the $\mathcal{H}_2$ norm of the approximation error by tangential interpolation conditions and also extend these results to the discrete-time case. We analyze whether it is reasonable to assume that lower-order models can always be approximated arbitrarily closely by imposing only first-order interpolation conditions. Finally, we analyze the $\mathcal{H}_2$ norm of the approximation error for a simple case in order to illustrate the complexity of the minimization problem.

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**MS106**

**Model Order Reduction Using New Concepts from Graph Theory and Numerical Analysis**

Although model order reduction techniques have been developed for many years and appear relatively mature, especially in the linear case, industrial requirements for such methods still have not been fulfilled. The problem of passivity has been addressed in recent years, but the work on passivity enforcement methods demonstrates there are still open issues. A similar observation holds for structure preserving methods, for which many research papers are being published currently. Suggested methods preserve only part of the structure, and other methods are needed to fill the gap. Another problematic issue is the case of multiple inputs and outputs, for which most of the standard methods become extremely inefficient. To solve all of these problems, and satisfy the needs of the electronics industry (one of the most stimulating environments for model order reduction), new concepts are needed. In this presentation, we will present novel techniques that bear the promise of being able to address the issues. Graph theoretic methods are used to drastically reduce extremely large multiport resistance and RC networks, whereas new ideas on spectral zeroes are used to obtain passivity and structure preserving methods.

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**MS107**

**A Scalable Coupling Toolkit for Multiresolution Models**

We present a toolkit for the development of scientific and engineering applications that involved the coupling of two or more numerical models. We address the scalability of the coupling interface as well as the flexible, reliability and robustness needed to accurately implement the interactions between the coupling components. We introduce the new interface to the Distributed Coupling Toolkit and its new functionality. We illustrate the DCT functionality using Earth Science Applications.

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**MS107**

**3D Partitioned FSI Simulation Using Level Set Function on Eulerian Mesh**

We develop a partitioned 3D FSI application code to combine advanced Eulerian fluid and Lagrangian structural solvers, i.e. parallelized CIP-FEM for high-speed flow analysis and structural elements considering large displacement/rotation increments for structural analysis. A large deformable interface is expressed as zero isosurface of the level set function on the fluid mesh, and the kinematical condition on the interface is handled. To confirm the validity of this code, unfolded airbag deployment is simulated.

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**MS107**

**Coupling Simulations in "Integrated Predictive Simulation System for Earthquake and Tsunami Disaster"**

This is a 5-year project from FY.2005, supported by Japanese Government, and will be the first integrate simulation system for prediction of earthquake and tsunami disasters using the Earth Simulator and T2K Open Supercomputers, which covers entire multi-scale processes such as plate deformation, dynamic fault rupture, seismic wave/tsunami propagation, and oscillation of buildings. In this talk, strategy for development of coupling codes and recent results of coupled simulations are presented.

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**MS107**

**Morfeus: A Pattern-Based Multiphysics Framework in Fortran 2003**

Over the past decade, scientific programmers have adopted many of the software engineering community's development practices, including languages, build systems, version control software and regression testing practices. Less influential have been their pre-development design practices such as design patterns and metrics. In particular, few researchers have taken up the challenge the originators of design patterns issued for experts to develop domain-specific patterns (Gamma et al., Design Patterns: Elements of Reusable Software, Addison-Wesley 1994). This talk presents Morfeus, a framework that employs several recently developed patterns that target multiphysics modeling (Rouson et al., ACM Trans. Math. Soft., in review). Morfeus is the Multiphysics Object-oriented Reconfigurable Fluid Environment for Unified Simulations. After presenting an overview of the system architecture and its application to problems ranging from quantum turbulence to magnetohydrodynamics and atmospheric dispersion, this talk will describe its implementation using the Fortran 2003 features that support object orientation and interoperability with C.

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**MS108**

**Experiences with Nonintrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Analysis and Design**

Non-intrusive polynomial chaos expansion (PCE) and stochastic collocation (SC) methods are attractive techniques for uncertainty quantification due to their abilities to produce functional representations of stochastic variability and to achieve exponential convergence rates in statistics of interest. Whereas PCE estimates coefficients for known orthogonal polynomial basis functions, SC forms

Lagrange interpolants for known coefficients. The latest results in comparing PCE/SC, tailoring for arbitrary random inputs, and embedding within design under uncertainty will be presented.

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**MS108**

**Applications of Polynomial Chaos to Ocean-acoustic Modeling**

We discuss an intrusive and non-intrusive application of polynomial chaos expansions for simulating uncertainty in ocean acoustics problems. One example uses a split-step algorithm to propagate an acoustic field through a waveguide within a narrow-angle parabolic approximation to the wave equation, with uncertainty in the sound speed field specified by a Karhunen-Loeve expansion. Another example uses a regression based approach to estimate the expansion coefficients for propagation with uncertainty in both source depth and sound speed. Work supported by the Office of Naval Research.

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**MS108**

**Uncertainty Quantification in Modular Structures through Concentration of Measure Inequalities**

We apply concentration-of-measure inequalities to the quantification of uncertainties in the performance of engineering systems. Specifically, we envision uncertainty quantification in the context of certification, i.e., as a tool for deciding whether a system is likely to perform safely and reliably within design specifications. We show that concentration-of-measure inequalities rigorously bound probabilities of failure and thus supply conservative certification criteria. In addition, they supply unambiguous quantitative definitions of terms such as margins, epistemic and aleatoric uncertainties, verification and validation measures, confidence factors, and others, as well as providing clear procedures for computing these quantities by means of concerted simulation and experimental campaigns. We also investigate the tightening of these inequalities and their extensions to systems characterized by multiple modules and scales. This is a joint work with Lenny Lucas, Michael Ortiz and Ufuk Topcu.

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**MS108**

**A Stochastic Dimension-reduction Method for Stochastic PDEs**

A dimension-reduction method is presented for solving stochastic PDEs. The solution is a multivariate function of the high-dimensional random input variables. High dimensional model representation is used to decompose this solution hierarchically into a sum of univariate, bivariate and higher-order component functions where each term in the representation reflects the individual or cooperative contributions of the random inputs upon the solution. The lower-order component functions are interpolated using adaptive sparse grid collocation method.

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**MS109**

**VisIt's Python Interface for Visualization and Analysis**

VisIt is a richly featured, open source visualization and analysis tool for scientific data. The program is fully scriptable through Python. In this talk, we will describe VisIt's capabilities and how to leverage them with Python.

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**MS109**

**Exploring Network Structure, Dynamics, and Function using NetworkX**

NetworkX is a Python language package for exploration and analysis of networks and network algorithms. The core package provides data structures for representing many types of networks, or graphs, including simple graphs, directed graphs, and graphs with parallel edges and self loops. The nodes in NetworkX graphs can be any (hashable) Python object and edges can contain arbitrary data; this flexibility makes NetworkX ideal for representing networks found in many different scientific fields. I will discuss some of our recent work studying synchronization of coupled oscillators to demonstrate how NetworkX enables research in the field of computational networks.

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**MS109**

**Matplotlib: Data Visualization in Python**

matplotlib is a 2D python graphics library. In combination with ipython, numpy and scipy, it provides a Matlab (TM)

like environment for scientific computing and visualization. In addition, it provides a class library which can be used to build applications on top of python's rich data structures and libraries. I will provide an overview of matplotlib's capabilities ranging from simple publication quality graphics with TeX-like support for mathematical expressions, to interactive graphics animating dynamical systems results.

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**MS109**

**An Efficient Computer Algebra System for Python**

The aim of this work is to provide a Computer Algebra System (CAS) for Python that will be used in Scientific Computation within Python: code generation, symbolic manipulations, etc. Sympycore, written in pure Python, is sufficiently efficient and robust for extension into a fully-featured CAS. Currently, Sympycore is comparable with the speed of many CAS-s that are implemented using a compiled language.

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**MS110**

**Methods of Data Assimilation in Chemistry and Transport Models**

The task of providing an optimal analysis of the state of the atmosphere requires the development of novel computational tools that facilitate an efficient integration of observational data into models. We discuss several new computational tools developed for the assimilation of chemical data into atmospheric models. The distinguishing feature of these models is the presence of stiff chemical interactions. The variational tools presented in this talk include automatic code generation of chemical adjoints, properties of adjoints for advection numerical schemes, calculation of energy singular vectors and their use in placing adaptive observations. Data assimilation results using the 4D-Var method are shown for several real test problems to illustrate the power of the proposed methods.

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**MS110**

**A Continuation Approach to Adjoint-based Observation Impact Estimation**

A continuation approach is introduced to analyze and develop adjoint-based methods for observation impact estimation in variational data assimilation. Second-order accurate measures consistent to 3DVAR/4DVAR analysis schemes are derived and issues related to the practical implementation are discussed. Equations of the forecast sensitivity with respect to the observation error variance are presented and a close relationship to the observation sensitivity is established. The potential use of the observed-minus-analysis increments to observation impact estimation is further investigated. Preliminary results are presented using NASA/GMAO GEOS-5 data assimilation system.

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**MS110**

**Optimal Solution Error Covariances in Variational Data Assimilation**

The problems of variational data assimilation (DA) may be formulated as optimal control problems to find some unknown parameters (initial and/or boundary conditions, right-hand-sides (forcings), distributed coefficients, etc.) The necessary optimality condition reduces the problem to the optimality system which contains all the available information. In practice the optimality system includes some input errors of different nature (background errors, observation errors, etc.). The error of the optimal solution (analysis) may be derived through the errors of the input data using the Hessian of the cost functional. For deterministic case it was done. If the errors of the input data are random and normally distributed, then for a linearized problem (tangent linear hypothesis) the covariance matrix of the optimal solution errors (analysis error covariance matrix) is given by the inverse of the Hessian of the cost functional. This result was given for a discretized problem. The same was shown for the continuous case, where a nonlinear evolution problem with an unknown initial condition was considered. Here we present an extension of the results from for the case of other model parameters (boundary conditions, coefficients, etc.) and show that in a nonlinear case the optimal solution error covariance operator can be approximated by the inverse Hessian of the auxiliary data assimilation problem based on the tangent linear model constraints. We also demonstrate that this approximation could be sufficiently accurate even though the tangent linear hypotheses is not valid

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**MS110**

**Model Reduction in 4D-Var Data Assimilation**

Strategies to achieve order reduction in four-dimensional variational data assimilation (4DVAR) search for an optimal low-rank state subspace for the analysis update. A common feature of the reduction methods proposed in atmospheric and oceanographic studies is that the identifi-

cation of the basis functions relies on the model dynamics only, without properly accounting for the specific details of the data assimilation system (DAS). In this study a general framework of the proper orthogonal decomposition (POD) method is considered and a cost-effective approach is proposed to incorporate DAS information into the orderreduction procedure.

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**MS111**

**A Study of Regularization and Boundary Integral Methods in Fully Lagrangian Kinetic Solvers**

Abstract not available at time of publication.

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**MS111**

**High-Order Discontinuous Galerkin Methods for MHD and Two-Fluid Plasma**

We present a class of high-order discontinuous Galerkin methods for solving three different fluid models of collisionless plasma: (1) MHD, (2) 5-moment two-fluid, and (3) 10-moment two-fluid. In the case of MHD, we develop an arbitrarily high-order constrained transport strategy for maintaining a divergence-free magnetic field. In the case of the 5- and 10-moment two-fluid equations, we consider a perfectly hyperbolic formulation of Maxwells equations for handling the divergence constraints. Finally, we present a heterogeneous multiscale method for coupling these various models, and apply this method to the problem of collisionless magnetic reconnection.

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**MS111**

**Modeling Multi-Ion Magnetohydrodynamics**

We solve the full set of magnetohydrodynamic equations with multiple ion fluids. The numerical difficulties and the algorithmic solutions are discussed: a total ion fluid is used in combination with the individual ion fluids, the source terms are evaluated with a point-implicit scheme using an analytic Jacobian, the multi-ion equations may be solved in a restricted region, and an artificial friction term is applied to limit the relative velocities of the ion fluids.

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**MS111**

**Novel Particle-In-Cell Simulation Methods in Heavy-Ion Fusion Science and Related Fields**

The Heavy Ion Fusion Science Virtual National Laboratory (HIFSVNL) has developed novel Particle-In-Cell (PIC) simulation methods for plasmas and beams, for high-energy density physics and inertial fusion energy: PIC with adaptive mesh refinement, a large-timestep mover for magnetized particles, and implicit methods; and for high energy physics: simulation in relativistically boosted frames, and a new relativistic leapfrog particle pusher. We will present the methods and example applications.

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**MS112**

**A Direct Factorization using Low Rank Submatrices as a Preconditioner for Acoustics and Electromechanics Applications**

We are interested in solving linear systems of equations that arise from acoustics and electromechanics applications using the boundary element formulation. The matrices are large and dense. They possess a nice property, for with a suitable blocking of the rows and columns, the off-diagonal submatrices are well approximated by low-rank submatrices. A "direct' factorization of the block matrix requires little more storage than the original, and has shown to require $O(1)$ iterations as a preconditioner to solve the linear

systems.

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**MS112**

**Hybrid Algebraic Multilevel Methods for Indefinite Problems**

In this talk we will consider algebraic multilevel methods for symmetric indefinite problems supplemented with a sparse direct solver. 3D problems are often too memory consuming to treat them with direct solvers. Instead preconditioned iterative methods are in favour. In particular AMG allows to reduce the initial system quickly to sizes where eventuelly direct methods are more attractive. We will consider large scale 3D problems such as the Helmholtz equation as well as saddle point problems (e.g. Stokes eqs.) to compare the hybrid approach with a pure multilevel method.

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**MS112**

**Investigations on Hybrid Solvers in the PhyLeas Project**

One route for solving efficiently large linear systems is the design of parallel hybrid linear system solvers which combine the robustness of direct methods with the implementation flexibility of iterative schemes. In this talk, we will present and discuss the various hybrid approaches that are studied in the framework of the PhyLeaS associate team that is a research initiative funded by the INRIA institute where French, German and American teams collaborated to develop such solvers.

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**MS112**

**A Hybrid Approach for Solving Large Sparse Least-Squares Problems**

We consider a hybrid approach for solving a large sparse least-squares problem, which is based on computing an exact orthogonal factorization of a submatrix of the given coefficient matrix. The submatrix is chosen so that the storage and time required to compute its orthogonal factorization and to employ the orthogonal factorization in the solution of the least-squares problem are small. Issues related to the choice of submatrices will be discussed.

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**MS113**

**Use of Chi-Square Test in the Analysis of Protein Alignments**

Results of DNA and protein alignment programs, BLAST and FASTA, are ordered by expectation values. This value depends on the size of the database and the types of sequences in the database. The chi-square statistical test is a possible way to determine the order of the alignments and find orthologs between the genomes sharing a common ancestor. The chi-square test leads to a more sensitive to determine orthologs. Advisors: Angela Shiflet, Wofford College and Gustavo Glusman, Institute for Systems Biology

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**MS113**

**Simulation of the Soft-Landing a Polyatomic Ion**

This past summer, I participated in research that involved colliding a charged molecule with a surface of hydrocarbon chains. In some cases we observed soft-landing, where the molecule stuck to the surface, but no chemical reaction took place. Soft-landing is important in the manufacturing of computer chips. We used computational techniques to simulate this process to better understand why the molecule sticks to or bounces off the surface. This understanding could help improve computer chips. Advisor: Angela Shiflet, Wofford College

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**MS113**

**Protein Sequence Coverage: Visualizing Tandem Mass Spectrometry Data with SVG**

The tool created for this project visualizes breadth and depth of protein coverage along full protein sequences. The software acts as a CGI; a simple URL with a custom-formatted query string serves as the request and a SVG document is the output. This dynamic approach replaces older static models and is capable of interactive visualization. Visualizing protein coverage allows for clear and convenient analysis of the extent of the protein identified by tandem mass spectra. Advisors: David L. Tabb and Matthew C. Chambers, Vanderbilt University Medical Center, Nashville, Tennessee

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**MS113**

**Predicting Foreign Exchange Rates: A Neural Network Approach**

Foreign exchange rates affect nearly every sector of global finance. In this project we try to create a model to forecast foreign exchange rates between the United States dol-

lar and eight other currencies. We explored linear versus nonlinear, regression versus neural networks, state space search versus parameter space search, and homogeneous versus heterogeneous data sets. We found an artificial neural network using a state-space search algorithm and the heterogeneous data set gave the best results. Advisor: Dr. Leong-Kwan Li (Hong Kong Baptist University)

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**MS113**

**Fast Evaluation on Adaptive Sparse Grids**

We consider the problem of evaluating a function in adaptive sparse grid space $G$ at many irregularly located points. Traversing all active basis functions incurs computational effort of $O(N)$, for a single point. Given algorithm evaluates a 2D function in $G$ (dimension $N$) at $N$ arbitrary points. Using a Segment Tree I reduce the computational effort of evaluation at $N$ points to $O(N \log^2 N)$.We generalize algorithm to higher dimensions. C++ implementation verifies our result. Advisors: Ralf Hiptmair and Gilela Widmer, ETH Zurich

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**MS114**

**Direct Numerical Simulation of Blood Flows in Abdominal Aortic Aneurysms**

The progression of abdominal aortic aneurysms (AAA) is strongly affected by blood flow shear stress. Blood flows through AAAs transit into turbulence under physiological flow conditions. This study aims to elucidate the impact of flow turbulence on surface shear stress and the AAA flow physics using direction numerical simulations. Results show that AAA flows are strongly affected by the size and length of the aneurysm and exhibit extremely rich dynamics.

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**MS114**

**Optimization and Virtual Interventions Improve Simulated Hemodynamics for Single Ventricle Heart Patients**

We will present blood flow simulations in the Fontan, a surgery performed on children with severe heart defects. First, patient specific simulations with detailed anatomy demonstrate the range of clinically relevant parameters that can be obtained through simulations. Second, we evaluate the performance of a new Y-graft design for the Fontan. The geometry of the Y-graft is systematically optimized using a surrogate-based derivative-free algorithm coupled to a three-dimensional Navier-Stokes flow solver.

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**MS114**

**Modeling Hemodynamics Past an Unoccluded and Partially Occluded Inferior Vena Cava Filter**

We use three-dimensional computational fluid dynamics to model the hemodynamics of an unoccluded and partially occluded TrapEase inferior vena cava filter. Flow disruption due to different sizes, shapes, and locations of blood clots is studied, and the clinical implications are assessed. Blood is modeled as a homogeneous, incompressible, Newtonian fluid, and the method of overset grids, as implemented in the Overture software framework, is used to solve the Navier-Stokes equations.

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**MS114**

**Modeling and Simulations of Fluid Structure Interactions in Left Atriumand Appendage**

In this talk, a novel numerical method for solving fluid and flexible structure interactions is introduced. The method is validated through rigorous convergence and accuracy tests. We focus our study on blood flows in the left atrium, one of the four chambers in the heart. Stable solutions are obtained at physiologic Reynolds numbers by applying pulmonary venous inflow, mitral valve outflow and appropriate constitutive equations to closely mimic the behaviors of biomaterials. Atrial contraction is also implemented as a time-dependent boundary condition to realistically describe the atrial wall muscle movements. From our study, the transmitral velocity, filling/emptying velocity ratio, durations and strengths of vortices are captured numerically for sinus rhythms (healthy heart beat) and they compare quite well with reported clinical studies.

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**MS115**

**An Approach of Full Diagonalization via Reduction of a Band Matrix; Performance and Scalability on a Multicore and Multiprocessor Environment**

In this multicore age, we need to modify or change the algorithm to utilize processor cores, cache and memory buses. As many know, the tridiagonalization phase of eigenvalue computation is costly, and its cost bounds by memory bandwidth. In this talk, another approach to diagonalize matrices will be argued from the viewpoint of automatic performance tuning. Furthermore performance on some multicore and multiprocessor systems will be reported.

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**MS115**

**Systematic Performance Evaluation for Numerical Algorithms of Linear Equations and Its Knowledge Discovery**

Systematical performance evaluation method for numerical algorithms of linear equations is proposed. An introduced computational system generates a performance information data set for a range of iterative solvers and preconditioning using a lot of typical test problems, and presents data visually allowing the relationships between the various algorithms and problems to be compared. Further, an application to automatic performance tuning is also introduced.

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**MS115**

**Robust and Efficient Parallel Preconditioning Methods with Extended Selective Blocking/Hierarchical Interface Decomposition for Multicore Architectures**

Development of robust and efficient parallel preconditioning method is a critical issue for scientific computing. Moreover, convergence of large-scale ill-conditioned problems strongly depends on the domain decomposition. In this presentation, author will describe robust and efficient preconditioning method based on extended selective blocking and extended HID (Hierarchical Interface Decomposition) for ill-conditioned problems. Efficiency and robustness of the developed methods are demonstrated on T2K Open Supercomputer (Tokyo) using Flat MPI and Hybrid parallel programming models.

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**MS115**

**Power-Efficient Computing with Automatic Tuning**

Methods of low-power computing on multi-core CPU machines enhanced by GPUs are discussed. The time and the power are modelized with referencing software parameters, and then the parameter values that gives the global minimum of time, power or energy is searched. We also discuss its automatic tuning, where the time and the power models are constructed automatically, and the minimization is done by the software itself.

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**MS116**

**On General Linear Time Stepping Methods**

The numerical solution of time-dependent partial differential equations and nonlinear hyperbolic conservation laws are of great practical. Traditionally, Runge-Kutta (RK) and linear multistep (LM) methods have been used for the time integration of ODEs, DAEs, and PDEs. However, LM methods have large stability limitations and RK methods develop order reduction. General linear methods (GLMs) are generalizations of both RK and LM methods and are aimed at improving their stability and accuracy properties. In this talk we present new developments for GLMs aimed at efficiently evolving in time hyperbolic conservation laws.

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**MS116**

**New Classes of Low-storage Runge-Kutta Methods**

Solution of partial differential equations by the method of lines requires the integration of large numbers of ordinary differential equations (ODEs). In such computations, storage requirements are typically one of the main considerations, especially if a high order ODE solver is required. We investigate Runge-Kutta methods that require only two storage locations per ODE. The low-storage properties of these methods can be related to certain sparse representations of their coefficients. This observation leads to new classes of low-storage methods with improved properties including, for instance, fourth order methods with four stages that use only two memory registers. Furthermore, the new class includes methods that retain the solution from the previous timestep or provide an error estimator, while still employing only two memory registers.

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**MS116**

**Extrapolated Implicit-explicit Time Stepping**

In this study we construct extrapolated implicit-explicit (IMEX) time stepping methods that allow to efficiently

solve problems with both stiff and non-stiff components. The proposed methods can provide high order discretizations of ODEs, index-1 DAEs, and PDEs via the method of lines. IMEX schemes based on extrapolation are simple to construct, easy to implement, and straightforward to parallelize. This work establishes the existence of perturbed asymptotic expansions of global errors and explains the convergence orders of these methods. Numerical results confirm the theoretical findings and illustrate the potential of these methods to solve multiphysics multiscale problems.

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**MS116**

**New Computational Approaches for the Simulation of Electrical Activity in Cardiac Tissue**

Mathematical models of electrical activity in cardiac tissue are often based on ordinary differential equations that describe the ionic currents at the cell level coupled with partial differential equations that describe how the electricity flows at the tissue level. The physiological accuracy of tissue-scale models is often limited by the efficiency of the numerical solution process. In this talk, I relate our experiences with numerical methods for the efficient solution of various cardiac electrophysiological models.

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**MS117**

**Parallel Mesh Smoothing using Mesquite and the ITAPS Interfaces**

Mesh quality improvement is often needed during the course of a parallel simulation as the mesh is adapted or moved to meet application needs. To meet this need, we have developed a parallel algorithm that builds on the state-of-the-art optimization-based smoothers in Mesquite. It this talk, we give an overview of the parallel algorithm, discuss the sychronization points necessary to ensure correct execution and our use of the ITAPS parallel interfaces, and show the scalability of the algorithm.

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**MS117**

**ITAPS Load Balancing Service**

Dynamic load-balancing is a data-management service that is critical to a wide range of unstructured and/or adaptive parallel applications. The Zoltan Library provides a suite of dynamic load-balancing tools. Access to Zoltan is now available through a common interface that supports interoperability within the ITAPS data model. In this presentation, we give a brief overview of the dynamic load-balancing service available through the ITAPS interface. We also give performance results for the ITAPS load-balancing service.

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**MS117**

**FronTier, A Meshed Lagrangian Interface Tracking Code and Its Scientific Applications**

This talk will introduce the renovated front tracking software library. We will show its numerical advantage as a meshed Lagrangian method: its geometry preservation through narrowly slotted Zalesak's disk undergoing many revolutions, its subgrid resolution, its reversal accuracy and its robust topological merging and bifurcation. We will introduce its template code and easy-to-call interface functions. We demonstrate the application of this library through simulations of fluid mixing, diesel jet, crystal formation, and other scientific problems.

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**MS117**

**ITAPS Based Software for Multiphase Flows in Nuclear Fusion Applications**

Novel numerical algorithms and parallel software for the simulation of multiphase hydro and MHD flows in nuclear fusion applications has been developed based on front tracking libraries of the SciDAC ITAPS Center. The software has been used for the simulation of the ablation of cryogenic pellets in the process of tokamak fueling and the implosion of plasma liners created by an array of converging supersonic plasma jets. Mathematical models, algorithms, and main simulation results will be discussed.

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**MS118**

**P-Multigrid Preconditioning for Finite-Element Electromagnetics Problems on Parallel Computers**

Multigrid methods are commonly used to solve the linear systems encountered in physical modeling. Order-based, or p multigrid, is particularly well-suited for use with hierarchical finite-element basis functions, and we will present the development and application of p-multigrid as a preconditioner for iterative methods in electromagnetics on parallel machines. When combined with other acceleration strategies, e.g., the A-V method, p-multigrid is shown to be an effective strategy for rapid solution of the finite-element matrix system.

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**MS118**

**Multigrid Algorithms for High-Order Discontinuous Galerkin Discretizations of the Compressible Navier-Stokes Equations**

Multigrid algorithms are developed for systems arising from high-order discontinuous Galerkin discretizations of the compressible Navier-Stokes equations. The algorithms are based on coupling both p- and h-multigrids (ph-multigrid). Two coupling strategies (two cycle types) are proposed. Both nonlinear and linear multigrid algorithms are considered as a solver. The linear variant is also used as a preconditioner for the Newton-GMRES solver. The performance of the algorithms are examined in solving the laminar flow around an airfoil configuration.

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**MS118**

**Two-level Optimized Schwarz Preconditioning for Spectral Element Based Magnetohydrodynamics**

A theoretical result for optimized Schwarz, presented in [SISC, 29(6),pp 2402–2425], enables the transformation of an existing Schwarz procedure to its optimized counterpart. In this work, it is shown how to modify a bilinear FEM based Schwarz preconditioning strategy to its optimized version. The latter is employed to precondition the spectral element pseudo Laplacian operator for the magnetohydrodynamic equations. In order to yield resolution independence in the Krylov iteration count a coarse solver is introduced.

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**MS118**

**Scalable Vlasov Solvers with High Order Methods**

In this paper, we will introduce our work on direct numerical simulation (DNS) of Vlasov equation, which is a substitution to the Particle-In-Cell (PIC) method for beam dynamic simulations. High Order Methods (HOM) have been used for discretization and Semi-Lagrange method for time integration. Domain decompositions in both physical and velocity spaces have been used for parallelization. Advantages of HOM and challenges will both be discussed. The new solvers can overcome some shortcomings of PIC codes.

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**MS119**

**Model Reduction for Linear Inverse Problems**

We discuss the application of system-theoretic model reduction methods based on balancing to large-scale inverse problems. Given a linear system described by the $m \times m$-transfer function $G(s)$ so that in frequency domain, inputs $u$ are mapped to outputs $y$ via $y(s) = G(s)u(s)$, we consider the question whether it is possible to reconstruct the input function $u$ from a given output function using system inversion, i.e., $u(s) = G^{-1}(s)y(s)$ when $G$ is replaced by a reduced-order model. We will discuss the implementation of balancing-related methods for the inversion of large-scale systems and error bounds for the input functions reconstructed using these methods.

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**MS119**

**Model Reduction for Multiscale Models of Textured Materials**

In two-level finite element simulations of textured materials, the stress-strain relationship at each quadrature point in a coarse-scale mesh is evaluated using a micro-scale finite element simulation. For even modest problem sizes, the cost of these micro-scale simulations becomes prohibitively expensive. In this talk, we discuss preliminary work on using model reduction to reduce the cost of the fine-scale computation in such simulations.

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**MS119**

**Empirical Interpolation for Nonlinear Model Order Reduction**

A variant of the empirical interpolation method (EIM) introduced by Barrault, Maday, Nguyen and Pattera in 2004 is presented and analyzed in matrix form. The method selects interpolation indices and constructs an interpolatory basis that is near optimal for approximation via interpolation from a specified finite dimensional subspace. Nonlinear functions are approximated via interpolation at the selected indices in the derived basis. Such an approximation may then be used in conjunction with a projection method to derive a reduced order nonlinear ODE from a given high order ODE. This approach has been highly successful in reducing computation time in the simulation of neural systems.

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**MS119**

**Model Reduction for Uncertainty Quantification and Decision-Making Under Uncertainty**

This talk will discuss formulations of model reduction problems for applications in uncertainty quantification. Key challenges include systems with input parameter spaces of very high dimension (infinite-dimensional parameters in some cases), and accounting for the statistical properties of interest in the system outputs. One possible strategy is a goal-oriented reduction approach; that is, we formulate the task of deriving the reduced model as an optimization problem. This provides an opportunity to derive models specifically tailored to the probabilistic problem at hand and adapted to the statistical quantities of ultimate interest.

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**MS120**

**A Multivariate Boolean Spectral Galerkin Method for Random Matrix Equations**

Nearly all tensor-product-based multivariate approximation methods suffer from an exponential increase in cost as the dimension increases. We develop an efficient multivariate spectral Galerkin projection for approximating the solution to a random matrix equation based on Boolean sums of tensor projections. In a similar spirit to nested sparse grid interpolation, the Boolean projection creates a nested set of projections that maintains the convergence properties of the tensor projections and alleviates the high cost associated with high dimensional problems. Additionally, the flexibility in the choice of bases allow for efficient computation of anisotropic problems.

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**MS120**

**Efficient Nonparametric Density Estimation for Randomly Perturbed Elliptic Problems**

We describe an efficient numerical method for nonparametric density estimation for quantities of interest computed from an elliptic problem with randomly perturbed parameters and data. The method employs the finite element method, non-overlapping domain decomposition, and the Neumann series for an invertible operator. We use an a posteriori error estimate using adjoint operators and variational analysis to distribute computational work in order to achieve a desired accuracy by an efficient distribution of computational resources.

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**MS120**

**Turbulent Mixing and Uncertainty Quantification: Simulations with Error Bars**

A clear sign of the importance given to simulation based design decisions is the increasing importance assigned to simmulation error bars. Campaigns for verification and validation (V&V) are now commonplace, and test for whether the mathematical equations have been solved correctly numerically (verification) and whether the mathematical equations accurately describe the physical problem to be solved (validation). Following the V&V campaigns is an uncertainty quantification (UQ) assessment, which attempts to determine error bars for simulations, as due to numerical approximations, phyiscal modeling approximations, or limited or inaccurate data. In this talk we will present examples originating in the modeling of turbulent mixing and turbulent combustion. The essentially statistical nature of the error bar analysis of simulation errors will be discussed.

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**MS120**

**Predictability and Reduced Order Modeling in Stochastic Reaction Networks**

Spectral methods are used for the dynamical analysis and

predictability in stochastic reaction networks described by a chemical master equation. First, reduced order modeling is accomplished by a Karhunen-Loève decomposition in time space. Further, Bayesian inference of polynomial chaos (PC) expansions allows representing the system state in the random space that corresponds to both intrinsic and parametric variabilities. Adaptive data clustering techniques are introduced to obtain mixture models of PC expansions that perform well for multimodal systems.

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**MS121**

**MPI and PETSc for Python**

MPI for Python provides support for classical MPI-1 features, like blocking/non-blocking point-to-point and collective communications, as well as more advanced MPI-2 features, like dynamic process management, remote memory access and parallel input/output. PETSc for Python provides access to PETSc and it is targeted to the parallel solution of linear and nonlinear problems within Python applications. We'll present both packages, discuss some design issues and illustrate the usage of basic and advanced features through simple examples.

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**MS121**

**Distributed Data Structures, Parallel Computing and IPython**

IPython is an open source project focused on interactive scientific computing. IPython includes an architecture for interactive parallel computing. This talk will describe how the abstractions in this architecture allow many different types of parallel computations to be performed in an interactive manner on everything from multicore CPUs to supercomputers. Both task and data parallel examples will be shown, with a focus on recently developed distributed memory arrays and hash tables.

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**MS121**

**Teaching Astronomical Data Analysis in Python**

We expect students in the physical sciences to become involved in research in their first or second undergraduate years, but today's research requires facility with a variety of advanced concepts, including computer programming, data handling, statistics, error analysis, modeling, and data presentation, each of which can occupy an entire course or more. One-on-one training by faculty is time-consuming, and in many cases research supervisors are not up-to-date on computational techniques. I have developed an undergraduate course in Astronomical Data Analysis whose goal is to allow students, upon completion, to knock on a researcher's door and say, "Put me to work, I'm plug-and-play." I will discuss course design with respect to this goal and how it addresses each of the topics above in one semester. I will present pros and cons of using both Interactive Data Language and Python as the base language for the class, and the experience of teaching the same material to the distinct populations of the Northeastern Ivy League and a large Southern state university, and to undergraduate and graduate students.

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**MS121**

**IPython: Components for Interactive Scientific Computing**

IPython provides components for interactive, exploratory and easy to use distributed and parallel computing. We discuss IPython's architecture and illustrate its tools, including multiple interfaces for interactive computing (text-based and graphical), components to build interactive environments, and a network abstraction of the Python virtual machine. We'll illustrate the benefits of the design by showing how the Vision system for graphical programming exposes high-level workflows for parallel computing with an IPython backend.

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**MS122**

**Challenges in Ensemble Kalman Data Assimilation for Atmospheric Chemical Transport Models**

In this study we investigate practical aspects of nonlinear ensemble data assimilation applied to atmospheric chemistry and transport models. We highlight the challenges encountered in this approach such as filter divergence and spurious corrections, and propose solutions to overcome them, such as background covariance inflation and filter localization. The predictability is further improved by including model parameters such as emission rates in the assimilation process. Results for a large scale simulation of air pollution in North-East United States illustrate the potential of nonlinear ensemble techniques to assimilate chemical observations.

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**MS122**

**An Unstructured Mesh POD Reduced Order 4D Var (ocean) Version of ICOM Model for Tsunami Modeling**

A Proper Orthogonal Decomposition reduced (by identifying the few most energetic modes in a sequence of snapshots from a time-dependent system), 4D-Var ocean model of ICOM is developed and applied to Tsunami modelling. We will progressively develop this model so that it can: 1)Predict the source location and regional wave heights from partial observational data sets. 2)Differentiate source type (e.g., line/point) and the effect of sea-bed perturbation on Tsunami propagation.

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**MS122**

**The Local Ensemble Transform Kalman Filter**

The Local Ensemble Transform Kalman Filter (LETKF) has proven to be a very accurate, model-independent data assimilation algorithm that can be implemented efficiently on highly parallel computer architectures. This talk will survey some of the latest results with the LETKF to global weather forecast models and an estuarine ocean model. I will also describe initial efforts to estimate and correct biases in atmospheric surface pressure observations.

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**MS122**

**Toward Assimilation of Sequences of Images in Numerical Models**

Since several decades satellites have been launched for the observation of the atmosphere and the ocean. They provide sequences of photographic images. These sequences of images contain information about the dynamics of the observed systems. We present an extension of the data assimilation techniques targeted to the assimilation of image sequences in geophysics. It relies mainly upon the definition of new observation operators that allow to compare model output with information extracted from the images.

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**MS123**

**Supporting Auto-tuning with Automatic Performance Analysis**

The complexity of high performance systems presents significant challenges for performance tuning of libraries and applications. In order to address this complexity, we designed an automatic performance analysis framework that extends Crays existing performance measurement and visualization tools and can be used by scientific library developers on their auto-tuning efforts. In this talk we will present the key aspects of this automatic performance analysis framework and its current development status.

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**MS123**

**Active Harmony: Online and Offline Autotuning**

Getting parallel programs to run well is a difficult, tedious, and time consuming task. In this talk I will present a system called Active Harmony that supports automated tuning of parallel programs. I will explain how Active Harmony can be used to automatically tune runtime parameters, and how it can be used to drive compiler optimizations. I will also present some performance results that show Harmony's auto tuning providing better results that manual efforts, and similar performance to exhaustive search of the parameter space.

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**MS123**

**Auto-tuning Scientifc Programs using Performance Counters**

Auto-tuning (or empirical optimization) is the process of generating libraries or applications tailored to the machine architecture and environment. This is done by generating multiple code variants and evaluating their performance

characteristics. The meaning of 'performance characteristics' depends on what the user is interested in - it could be elapsed time, cache misses, instructions per cycle, etc. In this talk, I will describe our tuning infrastructure and the use of PAPI to evaluate the characteristics of the generated code.

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**MS123**

**PAPI at PetaScale: Uniprocess Performance Measurement in Megaprocess Systems**

PAPI avoids most problems of large scale performance measurement tools by claiming to be a single-node measurement library, reporting performance counter values of a single cpu. But as systems scale beyond tens of thousands of processes, even tools such as PAPI can measurement resource contention between multiple cores on a single chip. This talk will present an overview of PAPI and explore the kinds of measurements available on newer multicore architectures.

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**MS124**

**Entropy Stable FEM Approximation of Compressible MHD**

A self-contained energy analysis [T. Barth, "On the Role of Involutions in Discontinuous Galerkin Discretization of Maxwell and MHD Systems', IMA Vol. in Math. and Apps., Vol. 142, 2005] is briefly outlined for the discontinuous Galerkin (DG) discretization [W. Reed and T. Hill, "Triangular mesh methods fo the neutron transport equation", Los Alamos Report, LA-UR-73-479, 1973] applied to the compressible magnetohydrodynamic (MHD) equations with solenoidally constrained magnetic induction field, div$B = 0$. Building upon symmetrization techniques for MHD developed by Godunov [S.K. Godunov, "The symmetric form of the MHD equations', Num. Meth. Mech. Cont. Media, 1972, pp. 26-34], this analysis quantitatively reveals why discretization of the MHD equations is fundamentally more demanding than either the Maxwell or hydrodynamic equations alone. Unlike standard hydrodynamics, the energy analysis for MHD reveals the subtle role of the solenoidal condition in obtaining global and elementwise local stability through

- strong or weak satisfaction of div$B = 0$ in element interiors
- strong or weak satisfaction of $[B \cdot n] = 0$ on element interfaces.

One immediate result from this theory are sufficient conditions to be imposed on numerical fluxes in hydrodynamics and magnetohydrodynamics so that energy stability and discrete cell entropy inequalities are rigorously obtained. The primary difficulty is actually constructing these stable approximation spaces on general element shapes. In this presentation, we report on current progress in this area and show numerical calculations of compressible MHD flow using the discontinuous Galerkin method together with high-order accurate approximation spaces.

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**MS124**

**Lagrangian Method for Warm Electrostatic Plasmas**

A numerical method is presented for warm electrostatic plasmas based on the Lagrangian formulation of the Vlasov-Poisson equations. The charge flow map is represented by quadrilateral panels in phase space. The particle-particle force is regularized and the panels are adaptively subdivided to resolve filamentation. Simulations are presented for the dynamics of a collisionless electron beam.

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**MS124**

**A Conservative High-Order Semi-Lagrangian Method for the Vlasov Equation**

We propose to solve Vlasov equation by a high order grid-based Eulerian approach. We design a class of conservative semi-Lagarangian numerical schemes that evolve point values, instead of integrated mass, for solving Vlasov equation with Strang splitting. Specifically, the proposed scheme uses Strang splitting to treat advection terms in different directions seperately; uses high order WENO (stands for weighted essentially non-oscillatory) reconstruction in each direction; and uses a conservative semi-Lagrangian scheme to update the point values of numerical solution. While the third, fifth, seventh and ninth order reconstructions are presented, the resulting scheme can be extended to arbitrary high order. As it is well known that WENO reconstructions have the advantages of being able to achieve high order accuracy in smooth part of the solution, while being able to capture sharp interface without oscillations. In our proposed scheme, we take those advantages. Moreover, the CFL time step restriction of regular finite difference or finite volume WENO scheme is removed, allowing cheaper and more flexible numerical realization. The quality of proposed methods are demonstrated through numerical experiments on basic test problems and on classical plasma simulation, such as Landau damping and two stream in-

stability. Our numerical results strongly suggest the usage of high order methods in space.

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**MS124**

**An Implicit Leapfrog Algorithm for Multi-scale Two-fluid Plasma Models**

An implicit leapfrog algorithm for solving the low-frequency two-fluid plasma model is proving effective for many plasma applications. The algorithm staggers center-of-mass flow velocity from other dependent fields, and von Neumann analysis shows that its numerical dispersion is i) comparable to time-centering for nearly perpendicular propagation and ii) greater for nearly parallel propagation at large time-step. Computational efficiency results from staggered advances and preconditioning developed for the combined spectral element/finite Fourier series spatial representation.

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**MS125**

**A Numerical and Analytical Study of Modeling Techniques for Solidification**

Abstract: The nonlinear and metastable nature of solidification has given rise to various numerical models that attempt to describe it. In this talk we provide a comparison of several computational models that describe solidification based on their ability to predict statistical properties of different materials. The results of numerical experiments and several extensions of the known modeling techniques are discussed. Advisors: Daniel M. Anderson, Maria Emeilianenko, Yuri Mishin, George Mason University

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**MS125**

**Identification of the Origins of Ligand-gated Ion-channels Using Global Ocean Survey Data**

Since Ligand-Gated Ion Channels (LGICs) are essential in higher organisms, the question arises as to where they come from. Using Global Ocean Survey (GOS) data, which consists of protein sequences of various simple aquatic organisms, we attempted to find any prokaryotic homologues of LGICs. Using computational tools that rely on sequence similarity analysis, we identified sequences that were similar to certain LGICs, showing a link between the LGICs and ion channels from simpler organisms. Advisors: Dr. Angela Shiflet, Wofford College, Andrew Pohorille, Exobiology Branch, NASA Ames Research Center

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**MS125**

**Modeling, Analysis and Computation of Fluid Structure Interaction Models for Biological Systems**

This undergraduate research presents mathematical models for the interaction of blood flow through arterial walls which are surrounded by cerebral spinal fluid. The blood pressure on the inner arterial wall is modeled using a Fourier Series approach. The outer part of the arterial wall and the surrounding cerebral spinal fluid will be coupled using appropriate partial differential equations. The fully coupled system will be analyzed using both analytical and computational tools. Applications of the model studied to intracranial saccular aneurysms will be presented. Advisors: Padmanabhan Seshaiyer, Javed Siddique George Mason University

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**MS125**

**Approximation of Hodgkin-Huxley Models by Exponential Integrate-and-Fire Models**

Effective strategies have been developed for finding the parameters in the recently proposed exponential integrate-and-fire point neuronal model that best approximates the membrane potential and firing rate dynamics of a given, detailed Hodgkin-Huxley-type, neuronal model. After implementing these strategies, we developed efficient adaptive algorithms for both systems, and analyzed the results of the computations. Further, we examined the same problem in the presence of an adaptive current. Advisor: Gregor Kovacic, Rensselaer Polytechnic Institute

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**MS125**

**The use of Surrogate Functions for Hybrid MINLP Particle Swarm Optimization**

Particle swarm optimization (PSO) is a population-based, heuristic optimization technique that is based on social behavior. The method has been shown to perform well on a variety of problems including those with nonconvex, nonsmooth objective functions. However, the method can be computationally expensive since many function calls are required to advance the swarm. We propose a hybrid algorithm using surrogate functions to serve as a more efficient information sharing medium within PSO. Advisors: Katie Fowler, Clarkson University and Thomas Hemker

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**MS125**

**Nonlocal Extensions of the Classical Phase Field Model**

The Classical Phase Field Model represents a coupling of an Allen-Cahn type nonlinear equation with a standard diffusion equation. This model has been proposed to describe non-isothermal phase separation in a pure substance. In this talk I will discuss an extension of that model which takes into account nonlocal effects by introducing a convolution term involving the phase ?eld variable. Results of simulations will be compared with the classical model to understand the effects of the nonlocal contribution. Advisor: Dr. Thomas Wanner, George Mason University

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**MS126**

**Utilizing Computer Models for Assessing Risk from Geophysical Hazards**

Risk assessment of volcanic pyroclastic flows is addressed through a combination of computer modeling, statistical modeling, and extreme-event probability computation. A computer model of the pyroclastic flows is utilized to provide the needed extrapolation to unseen parts of the hazard space. Statistical modeling of the available data is needed to determine the initializing distribution for exercise of the computer model. Direct simulation of rare events is prohibitively expensive, so an adaptively designed emulator is utilized.

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**MS126**

**Bayesian Multiresolution Methods for Spatial Inverse Problems**

The Bayesian statistical approach is a natural method for dealing with both the estimation of the inputs as well as quantification of the uncertainty around the estimated values, or for finding a range of plausible values consistent with the observed data. A process prior, such as a Markov random field, Gaussian process, or treed Gaussian process, is used to represent structure in the inputs, and the posterior distribution is estimated via Markov chain Monte Carlo. Multiresolution methods will be illustrated with several examples.

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**MS126**

**Nonparametric Bayesian Density Estimation in Hierarchical Engineered Systems**

We formulate a hierarchical Bayesian method for estimating polynomial chaos representations of random quantities from limited and noisy data. We introduce a reversible-jump Markov chain Monte Carlo scheme that simultaneously traverses polynomial degree and the corresponding spaces of coefficients, thus allowing infinitely parametric representations of the underlying random variables. Likelihood evaluations rely on a robust polynomial system solver. Examples center on the reliability and ageing of complex engineered systems, with extensions to general multivariate density estimation.

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**MS126**

**Bayesian Inference Using an Adaptive Sparse Grid Collocation Method**

We introduce a surrogate model for the likelihood calculation using adaptive hierarchical sparse grid collocation. This constructs an interpolant to the solution of the forward stochastic model in the prior space. Hierarchical Bayesian formulation is used and the unknown spatial model is represented as a convolution of a smooth kernel and Markov random field. The methodology results in sig-

nificant computational gains. The technique is assessed with a number of non-linear inverse problems.

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**MS127**

**Feedback Flow Controllers to Suppress Vortex Shedding Past Bluff-bodies**

In this talk, we present our progress to date for the design of feedback control laws to suppress vortex shedding behind a three-dimensional circular cylinder. We include a summary of our development of more accurate reduced-order modeling of the cylinder wake using the sensitivity of the proper orthogonal decomposition. In addition, we overview a number of strategies to incorporate Dirichlet boundary actuation and provide full-order closed-loop three-dimensional Navier-Stokes simulations at a range of Reynolds numbers.

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**MS127**

**Model Reduction in Cellular Neurophysiology**

Each cortical pyramidal neuron has over 100 branches with tens of synapses per branch. Partitioning each branch into 10 compartments, with 5 currents each, yields 50 variables per branch and results in a nonlinear dynamical system of 50000 equations. The challenge is to reduce the dimension of this system without sacrificing the rich spatiotemporal pattern of synaptic input. We report on our successful application of Proper Orthogonal Decomposition and the Empirical Interpolation Method.

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**MS127**

**Reduced-Order Modeling of Turbulent Flow**

Both accurate and computationally efficient simulations of turbulent flows are needed in important scientific and engineering applications, such as weather prediction and flow control. Reduced-order models represent natural choices in these applications. The fundamental challenge is to retain the physics of the underlying turbulent flow while keeping the computational cost at a minimum. In this talk, we present reduced-order modeling strategies synthesizing ideas originating from proper orthogonal decomposition and large eddy simulation of turbulent flows. In particular, we will present approaches based on the variational multiscale and dynamic subgrid-scale methods. Analysis and numerical illustrations of our methodology for both simplified settings and turbulent pipe flows will also be presented.

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**MS127**

**A Krylov $\mathcal{H}_\in$ Optimal Reduced Order Modeling Technique Applied to the Two-dimensional Linearized Shallow Water Equations: A Case Study**

Over the past few years the U.S. Navy's coastal ocean and riverine dynamical system modeling capabilities have taken large leaps forward. Direct numerical simulation using modeling tools is a standard approach and indeed one of the few available means to accurately predict environmental features that are influenced by riverine and near shore coastal processes. Reduced order modeling applied to these models is very promising and has enormous potential in the context of performing ensemble scenarios and data assimilation. The Krylov-based projection methods have emerged among the leading approaches for model reduction in large-scale settings, producing high quality models that satisfy (local) optimality conditions. In this talk, we present a case study in which we apply a Krylov $\mathcal{H}_\in$ optimal reduced order modeling technique to the two-dimensional linearized shallow water equations.

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**MS128**

**A Java Based Computational Framework for Simulation of Abnormal Thermo-Mechanical Environments**

A Java based computational framework is presented for simulations of abnormal thermo-mechanical environments. The coarse grain object oriented decomposition of the problem is based on physical descriptions of the relevant physical continuum processes (rather than the mathematics) for execution on massively parallel computational platforms. The framework is largely based on Eulerian region objects which defines the material (and associated mesh),

operators associated with transport processes and IO management. Communication between regions via MPI and multi-threading is supported through a region manager which handles the data for distributed and shared memory machines. Both traditional finite volume descriptions, finite element method and point wise Lagrangian descriptions of materials are supported as part of the region class, as well as interface classes to communicate information among them. Design choices for the data management and class construction will be shared with illustrative examples ranging from fundamental studies of strongly radiating turbulent multiphase flow and fluid-structure simulations, to applications of composite structure response to fire environments and post-detonation shock dispersal and ignition of metal particulate.

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**MS128**

**Fully Implicit Solution Framework for Scalable Earth System Models**

Major algorithmic challenges exist for the solution of Earth system problems such as coupled nonlinear physics, multiple disparate time scales, and scalability requirements. To access a range of solver capabilities needed to address these issues, a Fortran interface package of the Trilinos project is implemented within the High-order Method Modeling Environment (HOMME), a component option of the Community Atmosphere Model (CAM) that uses a cubed sphere grid and spectral element spatial discretization to achieve maximum scalability. By using the linearly implicit portion of the current semi-implicit solver in HOMME as a preconditioner, a fully implicit (FI) Jacobian-Free Newton-Krylov method is used to enhance the accuracy and efficiency of solution to a suite of shallow water test cases designed to evaluate various aspects of atmospheric modeling capability. Because FI provides a coherent nonlinear solution to all dependent variables, enhanced accuracy is achieved using a second order temporal discretization. Increased efficiency is attained for test case 2, where the steady state solution is not hindered by time step size constraints. The limitations of the gravity wave only based preconditioner with respect to efficiency and scalability will be discussed and improved preconditioning strategies will be outlined.

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**MS128**

**The General Curvilinear LAke Model (GCLAM) Computational Tool: An Application to the Valencia Lake, Venezuela**

In this work, we present a 3D computational tool called General Curvilinear Lake Model (GCLAM). The momentum equations describing the time development of a stratified fluid are solved using the GCLAM. This tool was tested in the Valencia Lake, Venezuela, in order to understand the three-dimensional circulation. Model results for different flow conditions are presented.

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**MS128**

**Development of a Cyberinfrastructure Environment for the General Curvilinear Ocean Model (GCOM)**

The long-term objective of this project is to develop an end-to-end gateway for the coastal ocean modeling and monitoring communities, based on the General Curvilinear Ocean Model (GCOM) and advanced cyberinfrastructure technologies. Primary activities include: development of a cyberinfrastructure to facilitate interactive and automated operation of the model, and to publish services; creation of simple user interfaces such as portals and command line tools to ease use; modularize GCOM to include new input models and to apply it to a variety of coastal regions; parallelize GCOM in order to utilize HPC/CI resources; and to publish GCOM services and results to be used by larger communities. GCOM solves 3-D, time-dependent, curvilinear flow equations to simulate stratified flows over uneven terrains.

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**MS129**

**Modeling of Fluctuations in Algorithm Refinement Methods**

We consider an approach for hybrid algorithms based on an adaptive mesh refinement paradigm. In this approach a hierarchical adaptive mesh refinement framework is used to embed a particle algorithm within the finest grid of the mesh hierarchy. The coupling between the particle region and the overlaying continuum grid is functionally equivalent to that between fine and coarse levels of mesh refinement. In this presentation we consider the role of fluctuations in this type of hybrid algorithm. In particular, we discuss the impact of fluctuations on the dynamics. We demonstrate that it is necessary to include a stochastic forcing term to model fluctuations at the continuum level to accurately capture the correct behavior of the system. We illustrate the role of fluctuations on two model problems. In the first we consider an excluded random walk model whose mean field behavior is given by the viscous Burgers' equation. The second example discusses a hybrid of direct simulation Monte Carlo with the compressible Navier Stokes equations. For the Navier Stokes equations we include stochastic fluxes as given by Landau-Lifshitz fluctuation Navier-Stokes equations. We will also discuss some of the issues in designing numerical methods for systems of this type.

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**MS129**

**Lattice-Boltzmann Simulations of Soft Matter**

On sufficiently large scales the effects of molecular-level fluctuations can be ignored, but at the colloidal scale and below, thermal fluctuations are an essential component of the dynamics. In this talk I will describe a lattice-Boltzmann approach to simulating fluid dynamics with thermal fluctuations. I will describe two different methods for coupling the solid and fluid phases, depending on the particle size, and give examples of each method.

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**MS129**

**A Higher-Order Approach to Fluid-Particle Coupling in Microscale Polymer Flows**

To simulate polymer flows in microscale environments for long time we have developed a numerical method that efficiently couples stochastic particle dynamics with an incompressible Navier-Stokes solver. Here, we examine the convergence properties of the stochastic particle solver alone, and demonstrate that it has second order convergence in both weak and strong senses, for the examples presented.

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**MS129**

**Particle-based Mesoscale Modeling of Complex Fluids: from Binary Mixtures to Polymer Solutions**

A particle-based simulation technique introduced by Kapral and Malevanets is generalized to model non-ideal fluids, binary and ternary mixtures. Transport coefficients and the equation of state for the fluid are derived, the phase diagram of the entropically driven de-mixing transition of the binary mixture is discussed. It is also shown how to model embedded wormlike chains with rigid bond constraints, thereby eliminating high frequency degrees of freedom and allowing the use of larger time steps.

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**MS130**

**Parameter Estimation and Uncertainty Apportionment using a Polynomial Chaos Approach**

Real time systems operate under parametric and external excitation uncertainties. The polynomial chaos approach has been shown to be more efficient than Monte Carlo for quantifying the effects of such uncertainties on the system response. In this talk we discuss efficient computational approaches for the application of polynomial chaos methodology in the simulation of stiff systems. The application of polynomial chaoses to the apportionment of uncertainties in three dimensional air quality models is explained. Data assimilation and parameter estimation techniques use information from observations of the real system together with imperfect model results to obtain improved estimates

of the model state and model parameters. We also discuss a parameter estimation approach that uses polynomial chaoses to propagate uncertainties and estimate error covariances in the extended Kalman filter framework. Parameter estimates are obtained in the form of a polynomial chaos expansion which carries information about the aposteriori probability density function.

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**MS130**

**Non-tensored Adaptive Strategies for Stochastic Multiwavelet Discretizations of Uncertainty Quantification Problems**

An adaptive multi-resolution analysis of problems with random parameters is proposed through intrusive Galerkin projections on stochastic multi-wavelet bases. The local resolution level is controlled using appropriate data structure and error estimators. Coarsening is included for time-dependent problems where the need for large resolution level evolves with time. We show that for parabolic and hyperbolic problems, adaptation can be applied both in time and space to obtain efficient computational strategies for complex nonlinear problems.

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**MS130**

**Generalised Polynomial Chaos for Oscillators with Random Parameters**

The mathematical modelling of dynamical systems often yields systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs). We consider systems, which exhibit a periodic solution for all physical parameters of a relevant set. In view of uncertainties, some parameters are replaced by random variables. Thus the corresponding periodic solution becomes a stochastic process. We apply the technique of the generalised polynomial chaos to resolve the stochastic model. Thereby, a Galerkin approach leads to larger coupled systems of ODEs or DAEs, respectively. We construct numerical methods for the solution of according periodic boundary value problems. The focus is on autonomous oscillators, where the period represents an additional unknown in the system. Furthermore, we discuss the local stability of corresponding periodic solutions. Results of numerical simulations using the constructed methods are presented.

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**MS130**

**Transition Pathways in Complex Systems**

Many problems in material sciences, physics, chemistry and biology can be abstractly formulated as a system that navigates over a complex energy landscape of high or infinite dimensions. Well-known examples include phase transitions of condensed matter, conformational changes of biomolecules, and chemical reactions. The energy landscape typically exhibits multiscale features, giving rise to the multiscale nature of the dynamics. The analysis of the transition pathways in such systems is a major challenge that we face in computational science. The string method proposed by E, Ren and Vanden-Eijnden is an effective way of identifying transition mechanisms and transition rates between metastable states in systems with complex energy landscapes. In this talk, I will discuss the theoretical background and algorithmic details of the method, as well as some applications.

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**MS131**

**Scientific Computing on Graphics Processors: FMM, FLAGON and Astrophysics**

The data parallel architectures of graphics processors require a fundamental rethinking of the algorithms commonly used in scientific computing. In particular, extracting meaningful performance increasingly requires the use of data structures that ensure that all data for computations is available without access to global memory. We have been exploring these issues both in the context of developing particular applications (fast multipole methods, particle in cell plasma codes, audio-visual signal processing), and in the context of the development of FLAGON, an open-source collection of modules and libraries for programming GPUs in Fortran 9X. Results from these efforts will be presented.

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**MS131**

**Many-core GPU Scientific Computing - Applications, Education, Tools, and Impact**

Abstract not available at time of publication.

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**MS131**

**Efficient Scheduling of Parallel Tasks in Dense Linear Algebra: PLASMA Framework**

PLASMA is a framework for a dense linear algebra library for multicore processors. The main objective of PLASMA is to address performance challenges of implementing compute intensive numerical routines on multicore hardware. PLASMA accomplishes this goal by utilizing novel algorithms, data structures and parallel scheduling methods. Here, main concepts behind the design of PLASMA are presented, followed by a discussion of different mechanisms for parallel task scheduling and different methods for expressing parallelism in software.

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**MS131**

**GPU Based High Performance Computing: A New Paradigm for Clinical Medical Imaging**

Medicine has been reshaped by new clinical imaging modalities, including four-dimensional computed imaging (4DCT) to study anatomical motion; and conebeam computed tomography (CBCT) for image guided procedures. Deformable image registration (DIR) can be used with these modalities, whereby target motion and changing physiology serve as inputs in treatment planning in radiation therapy. Due to long computation times, clinical applications of DIR have been limited to offline analysis. Graphics processing unit (GPU) computing is an emerging technology for general purpose computation, and is well suited for highly parallelized computing. Here use of GPU to extract tumor targets from 4DCT is presented.

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**MS132**

**Simulations of a Laboratory-scale Hydrogen Flame Stabilized on a Low Swirl Burner**

New combustion systems based on lean premixed combustion have the potential for dramatically reducing pollutant emissions in transportation systems and stationary power generation. However, lean premixed flames are highly susceptible to fluid-dynamical combustion instabilities making robust and reliable systems difficult to design. These difficulties are particularly challenging for hydrogen combustion because the flames are thermodiffusivley unstable. In this talk, we present simulations of a laboratory-scale hydrogen flame stabilized on a low swirl burner using detailed chemistry and transport without incorporating explicit models for turbulence or turbulence/chemistry interaction. We examine some of the basic properties of the flow field and the flame structure. We focus particularly on the cellular structures that arises from the thermodiffusive instability.

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**MS132**

**An Allspeed Method for Combustion**

In this talk, we present an allspeed algorithm for modeling combustion. In low-Mach number flows, the disparity of time scales between acoustic and convective motions introduces numerical challenges. A natural idea is therefore to separate the fast time scales to treat them implicitly, while the slower advective motions are treated explicitly or semi-implicitly. This method respects low-Mach number asymptotics but is suitable for any Mach number. We discuss benchmark results.

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**MS132**

**Simulation of Potential Detonations in Hydrogen Production Facilities Located Near Nuclear Reactors**

Generation IV Very High Temperature Reactors (VHTRs) are being designed to include hydrogen production capabilities. In this talk, we present the results of simulations modeling the risk associated with detonations in production facilities necessarily located near these reactors. In particular, we consider the effectiveness of earthen berms to deflect destructive waves away from reactor containments. To perform the simulations, we solve the reactive Euler equations on adaptively refined Cartesian grids using high resolution Godunov schemes and embedded boundary or mapped grid techniques to handle geometry. The codes EBChombo and ChomboClaw used to carry out the simulations will also be discussed.

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**MS132**

**The VTF - An Approach to Large-scale Simulation of Detonation-driven Fluid-Structure Interaction**

We describe the design concepts of the publicly available Virtual Test Facility (VTF) software that permits the effective computation of shock- and detonation-driven fluid-structure interaction problems. Several three-dimensional verification and validation computations involving elastic-plastic material behavior and fracture induced by detonation waves modeled with a simple volume burn model or with detailed chemical networks are presented. As large-scale example, we consider the plastic rupture of thin aluminum tubes due to interior detonations in ethylene-oxygen.

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**MS132**

**LES of Large Scale Hydrogen-Air Deflagrations and Jet Fires**

Large eddy simulation (LES) models of deflagrations and jet fires and their validations against large-scale experiments are described. Numerical simulations are compared against largest known experiments on hydrogen-air deflagration in: 20-m diameter hemisphere in the open atmosphere; 2.3-m diameter closed/vented sphere and non-uniform deflagrations in a closed cylinder of 5.7-m height and 1.5-m diameter; deflagrations in 78.5-m long tunnel. A LES model of high pressure hydrogen jet fire reproduced the largest experiment performed by Sandia.

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**MS133**

**Time-stepping Methods for Large Scale Differential Variational Inequalities (DVI) in Nonsmooth Dynamics**

We discuss recent advances in time-stepping methods for solving nonsmooth rigid body dynamics with contact and friction. The advantage of such methods is that they do not have to stop at every collision or stick-slip event while converging in a weak sense to the solution of the DVI. We discuss methods for solving the sub problems, which are optimization problems with conic constraints, arising at each time step. We particularly emphasize an algorithm that solves them in their dual cone complementarity form with a Gauss Seidel like iteration. We prove that the method is globally convergent. Through numerical experiments, we demonstrate that the method scales favorably with with an increasing size of the problem and we show that it is very competitive for the simulation of dense granular flow dynamics.

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**MS133**

**Geometric Integrators for Classical Molecular Dynamics: Theory and Application**

Trajectories generated by classical molecular dynamics (MD) are best interpreted in a statistical sense due to the weak definition of initial conditions and chaotic nature of the underlying equations of motion. For this reason, accuracy and efficiency of a time integration scheme should be measured with respect to statistical averages, rather than deviations from an "exact trajectory'. A practical MD time integrator must be both stable and statistically accurate, allowing for its use over long time intervals with large stepsizes. In this talk, I will survey some results from backward error analysis for geometric integrators and show how (under certain assumptions) these results can be applied to understanding the statistical properties of integrators for MD.

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**MS133**

**Uniform Convergence of Interlaced Euler Scheme for Stiff Systems of Stochastic Differential Equations**

Implicit methods for stochastic systems with multiple time scales modeled by SDEs are not effective in general. While implicit Euler has better stability properties over explicit Euler, it underestimates the stationary variance. We explore the idea of interlacing large implicit Euler steps with a sequence of small explicit Euler steps. We study the uniform convergence with respect to time scale separation parameter for linear systems and demonstrate that such interlacing could effectively deal with stiffness.

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**MS133**

**A Simple Technique for Solving Partial Differential Equations on Surfaces**

Many applications require the solution of time-dependent partial differential equations (PDEs) on surfaces or more general manifolds. Methods for treating such problems include surface parametrization, methods on triangulated surfaces and embedding techniques. This talk describes an embedding approach based on the closest point representation of the surface and describes some of its advantages over other embedding methods. Noteworthy features of the method are its generality with respect to the underlying surface and its simplicity. In particular, the method requires only minimal changes to the corresponding three-dimensional codes to treat the evolution of PDEs on surfaces.

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**MS133**

**Preconditioning for Linearly Implicit Methods in Geophysical Fluid Dynamics**

A Jacobian-Free Rosenbrock W-method is employed to solve the compressible Euler equations in a h-p adaptive discontinuous Galerkin solver. The latter is used for the simulation of atmospheric flows and the W-method requires no Newton type iterations. Moreover W-methods enable the use of inexact Jacobians: various preconditioning can therefore be constructed. Here we explore two-level preconditioning methods. They are applied polynomially in order to avoid the cost of the non-tensorizable inverses of the block Jacobians.

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**MS134**

**High-Productivity Supercomputing**

Metaprogramming GPU Architectures Tuning high-performance computational kernels relies on detailed ma-

chine knowledge, is error-prone and often tedious. Tuning is thus an attractive target for automation. This is "metaprogramming": Programs write and tune other programs. We present our approach to metaprogramming graphics processors from a scripting language. Our implementation of a Discontinuous Galerkin operator compiler and its supporting software illustrate how we obtain near-peak speed entirely from a high-productivity scripting language.

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**MS134**

**High-order Finite Elements in Extended Magnetohydrodynamics**

Extended magnetohydrodynamics (MHD) is a fluid model for plasmas that is characterized by anisotropic waves and extremely anisotropic heat fluxes. Resolving the anisotropies of both the waves and heat fluxes is a challenging problem that has been successfully met using high-order finite elements [Sovinec et.al., JCP 195, 355 (2004)]. Here, we present recent investigations improving the efficacy of high-order elements using the Mixed-Finite Element Method (MFEM), and improving the grid generation of distorted high-order elements.

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**MS134**

***hp*-Adaptive Finite Elements in a Parallel PDE Solver**

The *hp* version of the finite element method has been shown to have exponential rates of convergence with respect to the number of degrees of freedom, and consequently can be of optimal efficiency for many problems. Recently, *hp*-adaptivity has been added to the parallel elliptic partial differential equation solver PHAML. In this talk we will describe the method and present numerical results.

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**MS134**

**Architecture Aware Multigrid**

Multigrid methods are among the most efficient algorithms for solving elliptic PDE, however, the performance in real applications also depends on how well the algorithm is adapted to the computer architecture. We will discuss aspects of architecture aware implementations of multigrid including aspects such as using deep memory hierarchies, multicore processors and massively parallel systems.

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**MS134**

**True High-order Limiting for Conservation Laws Based on Total Variation Denoising**

This work presents a high-order limiting procedure, for discontinuous Galerkin approximations of conservation laws that avoids generation of non-physical oscillations in the presence of discontinuities. The idea is to regard the solution modes in troubled elements as input signals and to damp the oscillations by solving a non-linear local filter based on the Rudin-Osher-Fatemi denoising model. Numerical results demonstrate this procedure is capable of eliminating high frequencies in the solution and exhibiting good shock-capturing properties.

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**MS135**

**Intelligent Compilers**

The industry is now in agreement that the future of architecture design lies in multiple cores. As a consequence, all computer systems today, from embedded devices to petascale computing systems, are being developed using multicore processors. However, the wide disparity in hardware systems available has made it nearly impossible to write code that is portable in functionality while still taking advantage of the performance potential of each system. In this talk, we propose exploring the viability of developing intelligent compilers, focusing on key components that will allow application portability while still achieving high performance.

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**MS135**

**Proposal of Auto-Corrected IDR(s) for Highly Accurate Krylov Iterative Solvers Corrected**

Recently, the IDR(s) has been emerged as a high performance iterative solver, but it occasionally outputs incorrect solutions. To alleviate the problem, we propose an Auto-Corrcting type IDR(s). To avoid the incorrectness from the approximation of the original IDR(s), AC-IDR(s) predicts the occurrence of the incorrectness using the residual norm statistics and automatically replaces the approximation for the direct matrix vector multiplication. Numerical experiments show that the AC-IDR(s) solutions avoid the incorrectness in all cases.

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**MS135**

**Adaptive MPICollective Operations**

There are many algorithms to perform MPI collective operations. Algorithm performance depends on several variables: number of MPI processes, message size, interconnect, etc. We describe a method to automatically select the optimum communication algorithm at runtime. The method begins by searching the parameter space to find the critical variables for each MPI collective function. This information is used to create lookup tables or representative functions that can predict the optimum algorithm for each collective.

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**MS135**

**Automatic Tuning of MPI Applications with ASPhALT and Gravel**

MPI-based applications comprise much of the HPC workload of today and they can be difficult to code for performance. To address this issue, we present an Automatic System for Parallel AppLication Tuning (or ASPhALT) that relies on program transformations to improve performance. This talk will give an overview of ASPhALT and its lower-level messaging primitives called Gravel.

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**MS135**

**Toward Auto-tuned Cray Scientific Libraries**

For vendors like Cray, it has been more challenging to deliver tuned numerical libraries for commodity-based supercomputers. We address such problems through the automatic performance tuning framework designed to incorporate multiple tuning techniques and software tools together. Our flexible approach allows automatic tuning on different numerical software on different hardware configurations. In this talk, we describe the details of our software framework and our experience of tuning Cray Scientific Libraries (LibSci).

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**MS136**

**Domain Decomposition Solvers for Discontinuous Galerkin Discretization of the Time-Harmonic Maxwell Equations**

We report on the development of hybrid iterative/direct domain decomposition based algorithms for solving the undefinite sparse linear systems resulting from the discretization of the time-harmonic Maxwell equations using high order discontinuous Galerkin methods designed on unstructured tetrahedral meshes. The proposed algorithms combined a Schwarz-type algorithm where incoming characteristics based conditions are imposed at interfaces between neighboring subdomains, with a sparse direct method as the subdomain solver.

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**MS136**

**Multilevel Preconditioning Algorithms for Large-Scale Nonconvex PDE-Constrained Optimization**

Many interior-point optimization algorithms need to solve a sequence of closely related linear systems. The scalability of large-scale PDE-constrained optimizations ultimately depends on solving these symmetric linear systems quickly and reliably, which requires specialized iterative solvers. Novel strategies and algorithms will be presented in this talk to solve nonconvex optimization problems from three-dimensional PDE-constrained optimization with more than 30 million state variables and control variables on the desktop. Results for biomedical hyperthermia cancer simulations as well as other PDE examples will be presented.

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**MS136**

**Performance of a Parallel Algebraic Multilevel Preconditioner for Coupled Nonlinear PDE Systems: Transport/Reaction, Semiconductor Device, and MHD Applications**

This talk presents the performance of an algebraic multilevel preconditioner for the Newton-Krylov based solution of a challenging set of coupled nonlinear multiple-time-scale PDEs. These include transport / reaction, semiconductor device, and magnetohydrodynamics systems approximated by unstructured finite element methods. The algebraic multilevel preconditioner is based on a graph-based aggressive-coarsening aggregation method that uses the nonzero block structure of the Jacobian matrix. Results are presented for very large-scale linear systems solved on thousands of processors.

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**MS136**

**A Discontinuous Enrichment Method and Associated Domain Decomposition Solver for Acoustic Scattering in the Medium Frequency Regime**

The Discontinuous Enrichment Method (DEM) is a discretization method designed for the efficient solution of multi-scale problems. It is based on a hybrid variational formulation with Lagrange multipliers. In addition to an optional polynomial field, it employs free-space solutions of the governing differential equation for approximating large gradients or highly oscillatory components of the solution. It also relies on Lagrange multipliers to enforce a weak form of the inter-element continuity of the solution. In this talk, recent applications of DEM to the solution of acoustic scattering and fluid-structure interaction problems in the medium frequency regime are first discussed. Then, the case is made for a special class of iterative solvers that are tailored to this type of multi-scale discretization methods. To this effect, a nonoverlapping domain decomposition method is presented next for the solution of Helmholtz problems discretized by a variant of DEM obtained by dropping the optional polynomial field. In this new domain decomposition method, the subdomain degrees of freedom are eliminated by local static condensations to obtain an algebraic system of equations formulated in terms of the interface Lagrange multipliers only. As in the FETI-H and FETI-DPH domain decomposition methods for continuous Galerkin discretizations, this system of Lagrange multipliers is iteratively solved by a Krylov method equipped with both a local preconditioner based on subdomain data, and a global one using a coarse space. Numerical experiments performed for two- and three-dimensional acoustic scattering problems reveal that the proposed domain decomposition based iterative solver is scalable with respect to both the size of the global problem and the number of subdomains. Finally, the computational efficiency of the combined DEM and its associated domain decomposition based iterative solver is demonstrated for several benchark problems.

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**MS137**

**Accurate Interface Tracking in Multicomponent Flows via Space-time Adaptive hp-FEM**

We present a novel approach to interface tracking in multicomponent viscous incompressible flows based on space-time adaptive hp-FEM. The flow and the level set function are approximated on individual meshes that evolve in time independently of each other. Due to the local error control in both space and time, the method greatly reduces the inherent nonconservativity of the level set approach. The flow and the level set function are coupled monolithically. We show comparisons to methods working with fixed meshes and to space-time adaptive methods that approximate the flow and the level set function on the same mesh.

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**MS137**

**Towards Efficient DFT Electron Structure Calculation Using Adaptive Hp-FEM**

We study ab-initio electronic structure calculations in real space using density functional theory (DFT) and pseudopotentials. Essential ingredient of the methodology is the solution of eigenproblems of the Schroedinger equation. Originally, we have used standard (non-adaptive low-order) FEM for this purpose. We will describe the problems we run into and how the situation changed when we switched to adaptive hp-FEM (open source code Hermes). The most advanced calculation that we are going to present is the simultaneous solution of multiple eigenvalues in the context of the self-consistency cycle via adaptive multi-mesh hp-FEM. Numerical examples including comparisons to a single-mesh approach (multiple eigenfunctions resolved on the same mesh) will be presented.

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**MS137**

**Comparison of Different Refinement Criteria for Adaptive Mesh Refinement**

We have investigated and analyzed the grid convergence issues for adaptive mesh refinement (AMR) code using two different AMR packages. Ideally, AMR should achieve the same accuracy in refinement region as the corresponding fine uniform grid. We expect the results of an AMR grid should be better than the results of the coarse uniform grid

without local refinement. However, in one AMR package, we found numerical error with AMR is larger than without AMR. After detail analysis, we have found that the numerical solution at the coarse-fine interface between different levels of grid converges only in the first-order accuracy. Therefore, the error near the coarse-fine interface can quickly dominate the error in other regions if the coarse-fine interface is active and not covered by the fine grid. We propose, implement and compare several refinement criteria. Some of them can catch the large-error region near the coarse-fine interface and refine them with the fine grid.

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**MS137**

**Space-time Adaptive Hp-FEM for Time-dependent Multiphysics PDE Problems**

We present a novel space-time adaptive hp-FEM on dynamical meshes for time-dependent PDEs and multiphysics PDE problems. The method makes it possible to approximate various physical fields on individual meshes composed of different element types. The meshes evolve adaptively in time independently of each other, as required by the corresponding components of the approximation error. The splitting of meshes is particularly useful if the fields exhibit large qualitative differences. In the multiphysics case, the method is able to preserve exactly the coupling structure of the underlying PDE problem. The adaptivity algorithm is based on an estimate of the true error, not on the residuum or heuristic approaches such as steep gradients. For more details visit the home page of the open source project Hermes http://spilka.math.unr.edu/.

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**MS138**

**Hierarchical Models for Medical Imaging Computations**

Abstract not available at time of publication.

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**MS138**

**A Bayesian Approach to Probabilistic Sensitivity Analysis for Radiative Transfer Models**

Radiative Transfer Models (RTMs) simulate the interaction of light with a medium. Here, we focus on RTMs that model the light reflected from a vegetated region of the Earth. We study the Leaf Canopy Model (LCM) RTM, which takes as input leaf chemistry variables (e.g., chlorophyll and lignin) and canopy structural parameters (leaf area index and leaf angle distribution), and computes the upwelling radiation at the top of the canopy, which is ultimately observed by the satellite mounted sensor. We present a fully Bayesian approach to sensitivity analysis of computer models, and apply it to the LCM RTM to identify the inputs that have the greatest impact on the computed observation. The focus is on global sensitivity analysis, which studies how the RTM output changes as the inputs vary continuously according to a probability distribution over the input space. The influence of each input variable is captured through the posterior distributions for the "main effects' and "sensitivity indices'. A key advantage of the fully Bayesian approach is that it enables quantification of uncertainty associated with the sensitivity indices. We develop a Gaussian process approximation to the RTM output to enable efficient computation. The methodology is applied to the LCM with output obtained at specific wavelengths associated with bands of the satellite mounted sensors that are sensitive to vegetation.

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**MS138**

**Identification and Predition of Multiscale Dynamical Systems Using Bayesian Models**

This paper involves the derivation of reduced-order models for high-dimensional, multiscale dynamical systems. Such systems appear in several problems in computational physics and their direct simulation over long time periods is generally impractical or infeasible. Despite the high dimensionality of the observables , there exist a few generalized reaction coordinates that can be used to track the evolution of the system. Typical examples involve invariant manifolds in dynamical systems. Previous efforts in this direction have been dominated by POD-based models and variations which pose several limitations. In general, these reduced-order coordinates can vary with time in terms of their number and their relation with the observables. We propose a Bayesian nonparametric framework which can be trained with data generated by short bursts of simulation of the original system. At the core of the proposed methodology lie simple models in the nature of POD projections which are viewed as experts that explain (and potentially predict) the high dimensional observables in a partial and approximate manner. It is the combination of these experts through appropriate prior modeling that gives rise to a sparse and accurate lower-order representation.

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**MS138**

**Particle Filtering for Large Dimensional and Multimodal Sequential State Estimation Problems**

We study efficient importance sampling techniques for particle filtering when either (a) the observation likelihood is frequently multimodal or heavy-tailed, or (b) the state space dimension is large or both. When the likelihood is multimodal, but the state transition prior is narrow enough, the optimal importance density is usually unimodal. Under this assumption, many techniques have been proposed. But when the prior is broad, this assumption does not hold. We study how existing techniques can be generalized to situations where the optimal importance density is multimodal, but is unimodal conditioned on a part of the state vector. Sufficient conditions to test for the unimodality of this conditional posterior are derived. Our result is directly extendable to testing for unimodality of any posterior. Next we study how to reduce the importance sampling (IS) dimension of the problem by replacing IS by conditional posterior mode tracking for the part of the state space on which the state change is quite small. Applications in sensor networks and computer vision are demonstrated.

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**MS139**

**An Optimal Control Formulation of an Image Registration Problem**

The basic idea of image registration is to find a reasonable transformation which minimizes the difference between two given images. We derive an optimal control method for determining such a transformation; the approach is based on the grid deformation method and seeks to minimize an objective functional that measures the difference between the transformed image and the reference image. The existence of optimal transformation is proved as is the applicability of Lagrange multiplier method.

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**MS139**

**New Developments of the Optimal Control Approach to Registration**

We proposed an optimal control approach to image registration problem using a div-curl-ode system as constraint. Preliminary results in [1] and [2] and new developments will be discussed. [1] Liao et al, Optimal control approach to data set alignment, Applied Mathematics Letters, online 5 November 2007 [2] Chu et al, Adaptive Grid Generation Based Non-rigid Image Registration using Mutual Information for Breast MRI, Journal of Signal Processing Systems, online May 2008

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**MS139**

**Numerical Treatment of Landmark Constrained Image Registration**

Image registration is a challenging tasks within digital imaging. Given two images, the goal is to deform one one image such that it becomes similar to the other. The problem arises, when images taken from different objects, times, or devices need to be compared or fused. This talk presents approaches to constrained registration and in particular to landmark constraints. A general theoretical framework based on a variational approach is presented and supported by numerical treatment.

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**MS139**

**Deformable Multi-modal Image Registration by Maximizing Renyi's Statistical Dependence Measure**

We present a new framework for deformable multi-modal image registration. Our approach is based on Renyi's statistical dependence measure of two random variables/vectors, which is defined as the supreme of the functions of them in the space of measurable functions with with finite positive variance. We show that the space of functions in the definition can be restricted to the functions in the reproducing kernel Hilbert spaces associated with Gaussian kernels to simplify computation. Renyi's statistical dependence measure has certain desirable properties similar to mutual information (MI) that can be used for image registration. However, the computations in maximizing MI based algorithms are complex, and sensitive to the quantization of the intensities, because they require an estimation of the continuous joint probability density function (pdf), while using Renyi's statistical dependence measure we do not deal with the joint pdf itself but instead observed samples drawn independently. Experimental results are provided to show the effectiveness of the proposed method.

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**MS140**

**Massively Parallel Lattice Boltzmann Simulations for the Determination of Unstable Periodic Orbits in Turbulent Navier-Stokes Flow**

Unstable Periodic Orbits (UPOs) of chaotic and turbulent dynamical systems may be used in conjunction with the dynamical zeta function formalism to extract statistical in-

formation about the behavior of those systems. For this reason, the efficient computation of UPOs has gained importance and been addressed from various viewpoints in recent literature. In particular, approaches based on spectral representations of orbits lead to algorithms converging at a linear or close-to-linear rate with respect to orbit length. We present a new approach, based on a real-space representation of orbits, which preserves the favorable linear complexity of previous approaches but overcomes several limitations. Unlike spectral approaches, the real-space algorithm makes only weak assumptions for the smoothness of the initial condition, and is observed to converge even from initial conditions which are far from the final solution. In addition, storage requirements for the new approach are lower. We use this approach, together with the lattice Boltzmann equation, to extract UPOs of driven Navier-Stokes turbulence in two spatial dimensions.

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**MS140**

**Lattice Boltzmann Approaches to Electromagnetism and Magnetohydrodynamics**

The lattice Boltzmann approach has been extended to simulate resistive magnetohydrodynamics. The magnetic field is represented using a set of vector-valued distribution functions. The resulting algorithm has shown excellent parallel performance on many high performance computing platforms. The underlying kinetic equations have recently been shown to reproduce the full Maxwell equations plus Ohm's law, not just resistive magnetohydrodynamics. Many more phenomena can now be simulated, including electromagnetic waves, current-dependent resistivity, and ambipolar diffusion.

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**MS140**

**Coupled Lattice Boltzmann Molecular Dynamics Simulations: Translocation of Biopolymers Through Nanopores and Beyond**

We have recently developed a novel multiscale approach which concurrently couples a mesoscopic, lattice Boltzmann, fluid solvent with molecular motion. This scheme has been efficiently applied to the problem of biopolymer translocation through nanopores. Results from thousands of numerical simulations of long biopolymers up to 8000 monomers passing through pores of various sizes are presented. This multiscale methodology reproduces with remarkable accuracy the statistical scaling behavior of the translocation process and provides valuable insight into the cooperative aspects of biopolymer and hydrodynamic motion. Based on these results, we construct a phenomenological model which incorporates the statistical and dynamical features of the translocation process and predicts a power law dependence of the translocation time on the biopolymer length. In the case of wide pores, which are capable of hosting multiple polymer strands, there is clear evidence of folding quantization. The translocation proceeds through multi-folded configurations, characterized by a well-defined integer number of folds for which the rate of translocated beads at each time step is linearly correlated to the number of resident beads in the pore. As a result, the translocation time acquires a dependence on the average value of the folding number, which may result in a deviation from the single-exponent power-law characterizing the single-file translocation through narrow pores. The parallel implementation of this scheme exhibits excellent scalability on the BlueGene platform and improves the flexibility and efficiency of other complex multi-physics applications, such as hemodynamics, for which preliminary results will be presented.

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**MS140**

**A Lattice Boltzmann Approach to Fluctuating Multi-phase and Multi-component Fluid Simulations**

I present our recent progress on developing thermodynamically consistent simulations of fluctuating multi-phase and multi-component fluid mixtures. The Boltzmann equation describes the behavior of an ideal gas. The lattice Boltzmann method can be viewed as a discrete version of the Boltzmann equation. The usefulness of lattice Boltzmann method results from the fact that in the hydrodynamic limit (and for low Mach numbers) the behavior of an ideal gas is identical to that of a simple fluid. To extend the applicability of the lattice Boltzmann method several extensions have been proposed: **Multi-component mixtures**: By allowing different cross-sections for the collisions between different species we recover non-Fickian diffusion, equivalent to the Stefan Maxwell diffusion model. **Non ideal fluids**: It has long been known that the lattice Boltzmann method can be extended to non-ideal fluids. We show how one can derive a consistent approach to including averaged interactions which can be derived from an underlying free energy. We verify that these interactions lead to the correct equilibrium behavior of a phase-separating fluid mixture with a constant chemical potential and divergence free pressure. **Fluctuations**: The Boltzmann equation deals with expectation values and is therefore non-noisy. This can be a problem for situations where fluctuations are important, *e.g.* dynamics near a critical point or diffusion

of suspended colloidal particles. We discuss how one can incorporate these fluctuations by introducing a fluctuating collision operator.

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**MS141**

**Recent Results in Passivity Preserving Model Reduction**

A basic problem is the electronics industry consists in replacing a passive (mostly linear) circuit with one of lower complexity. There are a number of methods which achieve this goal. However a systematic way of synthesizing the obtained low complexity circuit by means of resistors, inductors and capacitors, is missing. In this talk we will address the combined passivity preserving reduction and synthesis problem and present preliminary results for its solution.

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**MS141**

**Optimal Krylov Subspace-Based Model Order Reduction of Large-Scale RCL Networks**

It is well known that the Lanczos process can be used to efficiently compute Padé reduced-order models of large-scale linear dynamical systems. While these models have optimal accuracy in the sense of Padé approximation, in general they do not preserve other important properties, such as stability and passivity, of the original system. For the case of systems describing RCL networks, this has led to the development of other Krylov subspace-based reduction techniques that do preserve the crucial properties of the original systems. However, these algorithms have no longer optimal approximation accuracy. In this talk, we discuss some recent progress on the problem of constructing structure-preserving Krylov subspace-based reduced-order models that have optimal approximation accuracy.

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**MS141**

**Passivity-Preserving Balanced Truncation for Electrical Circuits**

We introduce a generalization of the model reduction by passivity-preserving balanced truncation of descriptor systems. We especially apply this method to the equations of linear RCL circuits. It is shown that the special structure of circuit equations can be used to reduce the numerical effort for the computation. We further consider the realization of the reduced-order model as a electrical circuit. This allows the back interpretation of the reduced-order model as an electrical circuit.

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**MS141**

**Reduction for Computing Cell-Averaged Behavior from Biochemical Kinetics Models**

Transduction or regulatory pathways in biological cells are often modeled by systems of differential equations that describe how concentrations of biochemical species evolve in time. These biochemical kinetic models describe single cell behavior, but data available for comparison is often based on experiments that average over tens of thousands of cells. In this talk we discuss the specialized problems in trying to use model reduction to reduce the cost of computing cell-averaged quantities from single cell biochemical kinetics models.

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**MS142**

**Onion-type Hybrid Models: From Atomistic Molecular Dynamics to Continuum Hydrodynamics, Passing Through Adaptive Coarse-graining**

The final goal of multiscale models based on domain decomposition, is to retain full atomistic detail only where needed (within a region of interest), while using a coarse-grained model to introduce the essential information about the surroundings dynamics. Importantly, the atomistic region becomes an open sub-system which exchanges mass, momentum and energy with the exterior. A proper hydrodynamic description of such exchange needs to be based on flux balance and can be solved using an hybrid molecular-continuum description (hybrid MD) [1,2]. However, molecule exchange across the hybrid interface becomes a complicated task as one deals with more complicated molecules, essentially owing to larger steric hindrance. A way to solve this bottleneck is to combine hybrid MD with adaptive coarse-graining. The setup resembles the layers of an onion [3]: the atomistic model lies at the core, surrounded by a thermodynamically compatible coarse-grained model, which interfaces with a continuum description of the liquid (maybe also including hydrodynamic fluctuations). Finally, open boundary conditions for the continuum description [4] allow evacuation of (shear, heat or sound) waves out of the whole system, and let it behave in a grand-canonical way, in contact with the prescribed outer thermodynamic state. [1] G. De Fabritiis, R. Delgado-Buscalioni and P. Coveney, Phys. Rev. Lett.97, 134501 (2006) [2] R .Delgado-Buscalioni and G. De Fabritiis, Phys. Rev. E 76, 036709 (2007) [3] R. Delgado-Buscalioni, K. Kremer and M. Praprotnik, J. Chem. Phys. 128, 114110 (2008) [4] R. Delgado-Buscalioni, A. Dejoan, Non-reflecting boundaries for ultrasound in fluctuating hydrodynamics of open systems, Phys. Rev. E, in press, (2008)

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**MS142**

**A Hybrid Continuum-Particle Method for Polymer Flows**

Particle methods have been used for modeling polymer chains in flow for some time. Typically, Molecular Dynamics (MD) is used for the polymer chains, and the solvent is modeled with a mesoscopic method. We use a recently-developed Event-Driven Molecular Dynamics (EDMD) [A. Donev and A. L. Garcia and B. J. Alder, J. Comp. Phys., 227(4), 2644-2665, 2008] algorithm in which the polymers are modeled as chains of hard spheres and the solvent is modeled using a dense-fluid generalization of the Direct Simulation Monte Carlo (DSMC) method [Phys. Rev. Lett., 101, 075902, 2008]. Even with all of the speedup compared to brute-force MD the algorithm is still time-consuming due to the large number of solvent particles necessary to fill the computational domain. It is natural to restrict the particle model only to regions close to a polymer chain and use a lower-resolution continuum model elsewhere. We present a hybrid method that couples an explicit fluctuating compressible Navier-Stokes solver with the particle method. The coupling is flux-based and generalizes previous work [J. B. Bell and A. Garcia and S. A. Williams, SIAM Multiscale Modeling and Simulation, 6, 1256-1280, 2008] to dense fluids as appropriate for polymer problems. We investigate the accuracy of the coupling scheme for both an ideal and a non-ideal fluid and validate the method's ability to correctly reproduce fluctuations as well as hydrodynamic interactions. Note: This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-404680).

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**MS142**

**Multiscale Modeling in Complex Fluids and Soft Matter**

Understanding flow phenomena in complex fluids and biomedical applications require the use of multiscale modeling approaches. We present the triple-decker algorithm, a hybrid method based on coupling atomistic, mesoscopic and continuum methods, which correspond to the Molecular Dynamics (MD), the Dissipative Particle Dynamics (DPD), and the incompressible Navier-Stokes (NS), respectively. MD, DPD, and NS are formulated in separate subdomains and are coupled via an overlapping region by communicating state information at the sub-domain boundaries. The flexibility of this method allows for an efficient spatiotemporal decoupling. In addition, the method is not restricted to only three descriptions coupling, and can be analogously applied to MD-DPD, DPD-NS or coupling together two levels of coarse-graining descriptions. We will provide results which involve coarse-grained models of flexible polymers and red blood cells.

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**MS142**

**Multiscale Simulations of Water**

We present algorithms for the coupling of atomistic, mesoscopic and continuum descriptions of liquid water. We discuss the requirements for multiscale simulations of polar, polyatomic molecules such as water and discuss extensions to aqueous solutions of other polyatomic molecules.

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**MS143**

**Efficient Low-rank Separated Approximation of a Class of High-dimensional Uncertain Systems**

Separated representations have proven efficient to relax the curse of dimensionality associated with approximation of high-dimensional functions. Such representations can be considered as a generalization of singular value decompositions for dimensions larger than 2 without being optimal. The alternate least-squares (ALS) algorithm has been used to construct such separated representations; it has been shown that the computational cost associated with such procedure formally grows linearly with respect to the dimensionality of the function. The authors have successfully extended the separated representation formalism for a lowrank approximation to the solution of partial differential equations with highdimensional input data based on the ALS algorithm. In the present study, we present a more efficient way of constructing the separated approximation for the case of linear elliptic stochastic PDEs with a high-dimensional multiplicative noise. The proposed approach is based on an alternating Rayleigh-Ritz variational formulation of random linear system of equations arising from the spatial discretization of the problem. The superiority of the proposed scheme over the traditional ALS approach for this class of problems will be demonstrated. Finally, different aspects of the algorithm will be explored through its application to different problems in mechanics.

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**MS143**

**A Random Matrix Approach to Multiscale Me-**

**chanics**

We describe a probabilistic construction for a certain class if random matrices that are typical in multiscale mechanics. These matrices are bounded from above and below over a compact subset of the set of symmetric positive definite matrices. We construct a probability measure over the set of these matrices using the maximum entropy principle with suitable constraints and develop sampling algorithms for synthesizing numerical realizations of these matrices which can then be used as constitutive matrices in suitable applications in mechanics.

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**MS143**
**Inverse Modeling of Two-phase Flow Using Moment Equations**

We present an inversion algorithm for immiscible two phase flow in heterogeneous porous formations. The first two statistical moments of the permeability field are conditioned directly using saturation measurments and phase flow rates at wells. The forward problem consists of solving the statistical moments equations that govern the flow field and the transport. A Kriging based approach is used to update the permeability moments. Examples of immiscible two-phase flow in the quarter-five-spot configuration are presented and compared with standard Monte Carlo Simulation.

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**MS143**
**Finite Element Approximations of the Darcy's Equation in Random Porous Media Without Uniform Ellipticity and Continuity**

In this talk we consider a stochastic Darcy's pressure equation with log-normal permeability and random right-hand side forcing term. To accommodate the lack of ellipticity, singular forcing terms, and general representations of the permeability stochastic fields, we introduce new continuous and discrete weak formulations involving distinct spaces for the solution and the test functions. We present inf-sup conditions, well-posedness, a priori error estimates and numerical experiments.

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**MS144**
**Computational Finance Applications using CUDA**

In this talk I will discuss the parallelisation of financial Monte Carlo and finite difference calculations on NVIDIA GPUs. The trivially-parallel Monte Carlo application achieves excellent speed-up using multi-threading to hide pipeline stalls and memory access latencies. The finite difference application also achieves good performance for both explicit and implicit time-marching, using an approach taken from distributed-memory parallelisation.

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**MS144**
**GPU Cluster Computing for FEM**

This presentation explores GPU acceleration of parallel multigrid solvers for Finite Element simulations on commodity based clusters. The integration, based on a mixed precision iterative refinement scheme, is minimally invasive in the sense that it requires no changes to application code: Hardware acceleration is completely encapsulated from the application level. We demonstrate good scalability and accurate results for the prototypical Poisson problem and applications in linearised elasticity and fluid dynamics. Finally, we derive a performance model to accurately estimate the achievable speed-up.

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**MS144**
**Extracting Parallelism from Financial Applications with SIMD, Multicore, and Manycore**

This presentation starts with the evolution of computational requirements in quantitative finance, and then takes a popular numerical method, Monte Carlo Simulation as an example to demonstrate how to extract parallelism using conventional high level languages such as C/C++ to take advantage of SIMD, multicore and manycore technology. It demonstrates a standard extension that enables this method to take advantage of an X86-based manycore technology. At the same time, the programming model and software development tools and application performance issues for this environment will be discussed in detail. In the end, the authors will provide a brief outlook on how to extend this programming model to other popular kernels in the financial risk management calculations.

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**MS144**
**Fluid Flow Simulations on Roadrunner**

We present results from a parallel hybrid implementation of a compressible Navier-Stokes solver on Roadrunner. This

is the first implementation of a large structured-grid fluid dynamics code on this architecture. In contrast to other applications that have been ported to the Cell, codes of this type are typically limited by memory bandwidth. Nevertheless, the memory subsystem of the CBE, coupled with explicit memory management, allows order of magnitude speed improvement and effective memory bandwidths approaching 50% of peak. Both memory spaces of the hybrid architecture are used to maximize performance and mitigate the imbalance between internode communication and computation speed.

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**MS145**

**Teaching Numerical Linear Algebra with CSE Applications**

This talk is concerned with teaching of numerical linear algebra, at both undergraduate and graduate levels. The following topics will be covered : the role of numerical linear algebra in the mathematics, computer science and engineering curricula ; suggested syllabuses; prerequisites for studies of numerical linear algebra ; and, special tips for teaching numerical linear algebra in class rooms. Examples from personal experience will be given, whenever appropriate. Some details of this talk can be found in my web page: www.math.niu.edu/ dattab

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**MS145**

**Programming and Algorithms for CSE Undergraduate and Beginning Graduate Students**

One of the fundamental building blocks of CSE (both at undergraduate and graduate levels) is the ability to write software of moderate complexity and to perform analyzes to chose appropriately among algorithms. Getting students to an appropriate level of proficiency is difficult in the one or two course that such degree programs allow. However, engineers and scientist do write software. Thus, it is imperative that we provide them with principles of good software engineering.

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**MS145**

**Integrating CSE Into the Liberal Arts Curriculum**

The pervasiveness of information technology today provides opportunities to integrate Computational Science into educational programs well beyond the common fields of chemistry, physics, biology, economics, mathematics and computer science. The challenge is overcoming perceptions among students and instructors in these non-traditional and broader disciplines regarding computational science. This presentation will focus on efforts and strategies to encourage adoption across disciplines ranging from art to communication to religion and ethics.

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**MS145**

**Using CSE Dynamic Simulations to Present Applied Mathematics to Undergraduates**

Providing opportunities for advanced undergraduate professional development is a clear challenge in CSE education. Integration of non-trivial applied mathematics must be accomplished while challenging students to question modeling assumptions, computing methods, and solution accuracy. The dynamic simulation of an aerospace vehicle structural panel in supersonic flow is presented as a useful course module. Such modules foster professionalism and may be used in collaborative CSE curricula among a number of cooperating institutions and programs.

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**MS146**

**A-posteriori Based Stabilized DG Schemes for Evolution Equations**

In this talk we present an hp-adaptive scheme in space and time for the discretization of systems of evolution equations

$$\partial_t U(t,x) + \nabla \cdot \Big( F(U(t,x),t,x) + a(U(t,x),t,x)\nabla U(t,x) \Big) = S(U(t,x),t,x)$$

We base our method on the higher order Discontinuous Galerkin method in space and explicit methods in time using general parallel grid structured with h-adaptivity. Our focus is on the convection dominated case, so we discuss approaches for gradient limiting and p-adaptivity for stabilizing the scheme in the regions of strong gradients or discontinueties. The basis of the hp-adptivity is an a-posteriori error estimate for the semi-discrete method. For the implementation of the scheme we use the free software package DUNE (dune.mathematik.uni-freiburg.de).

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**MS146**

**Space and Time Adaptivity for Finite Volume Methods**

Adaptivity in space and time are introduced to control the error in the numerical solution of parabolic and hyperbolic partial differential equations and similar equations. The equations are discretized in space by a finite volume method and in time by a linear multistep method. The computational grid is refined and coarsened dynamically in blocks. There are jumps in the step size only at the block boundaries. The local truncation error is estimated and the step size and the time step are chosen to satisfy a bound on this error. The method is applied to the Euler equation of fluid flow with and without shocks, the chemical master equation, and its approximation the Fokker-Planck

equation.

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**MS146**

**Multiscale Astrophysics of Thermonuclear Supernova Explosions**

Vastly different spatial and temporal scales characteristic of astrophysics put extreme demands on computing facilities, both in terms of hardware use and software complexity. This makes computational astrophysics an excellent technology driver. Its diversity leads to new and welcomes existing solutions originally developed in different context, offering synergy and aiding in solving general large scale, multiscale and multiphysics problems. I will illustrate such astrophysics applications with examples of radiative shocks, stellar mergers, and thermonuclear supernovae.

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**MS147**

**Multilevel Adaptive Monte Carlo Sampling for Inverse Problems**

Over the past few decades, efficient and robust multilevel solvers have been developed for a variety of applications which range from medical tomography to flow in porous media. Recent success of these multilevel solvers is due to the development of general multiscale concepts such as operator-induced variational coarsening. This approach implicitly treats the multiscale aspects of the fine-scale model in its generation of successively coarser representations. Clearly such solvers can be used as a "black box" (within an MCMC scheme, for example) for inferring unknown parameters or initial conditions in inverse problems. While computational efficiency has been the primary motivation for the development of such multilevel solvers, it is hard to resist the temptation of prying into these solvers so that the coarser representations can be used to help guide the posterior sampling. In this talk we explore sequential and Markov chain Monte Carlo methods for exploiting the implicit coarsened representations within a mulitlevel solver to speed up posterior sampling.

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**MS147**

**Bayesian Functional Data Analysis for Computer Model**

Abstract not available at time of publication.

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**MS147**

**Bayesian Functional Data Analysis for Computer Model Validation**

Functional data analysis (FDA) inference on curves or functions has wide application in statistics. An example of considerable recent interest arises when considering computer models of processes; the output of such models is a function over the space of inputs of the computer model. The output is functional data in many contexts, such as when the output is a function of time, a surface, etc. A nonparametric Bayesian statistics approach, utilizing separable Gaussian Stochastic Process as the prior distribution for functions, is a natural choice for smooth functions with a manageable (time) dimension. However, direct use of separable Gaussian stochastic processes is inadequate for irregular functions, and can be computationally infeasible for high dimensional functions. In this talk, we will develop and extend Bayesian FDA approaches for complex computer model validation, tailored to interdisciplinary problems in engineering and the environment.

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**MS148**
**Adaptive Mesh Refinement for Image Registration**

Already for reasonable sized 3D images, image registration becomes a computationally intensive task. Here, we introduce and explore the concept of method for registration which drastically reduces the number of processed data and thus the computational costs. We present a suitable optimization technique. Furthermore, we demonstrate the performance of the new approach by academic as well as real life examples.

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**MS148**
**Elastic Registration Using Dendro**

Image registration is a challenging problem for several reasons: the choice of the image similarity functional, the regularization, and the numerical solution of the chosen formulation. Here, we are interested in numerical algorithms for variational image registration. As a model problem, we consider 3D L2 elastically-regularized registration. This is a nonlinear non-convex variational problem. We address some of the computational challenges involved in solving the problem using (a) Multigrid and (b) Adaptivity. In our work we use 'Dendro', a parallel geometric multigrid algorithm for finite elements on octree meshes that has scaled to billions of elements on thousands of processors.

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**MS148**
**Learning to Segment in a Bayesian Framework**

Image segmentation is often uses a generative probabilistic model for the image. But there are many segmentation problems where generative models are too complicated to create. For such problems it is simpler to use discriminative models – these models directly model the posterior instead of using the Bayes theorem to calculate the posterior from the generative model. This talk presents the results of segmenting cardiac ultrasound data using a discriminative model.

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**MS148**
**Estimation of Vector Fields in Inequality Constrained Variational Problems for Image Segmentation and Registration**

We develop coupled partial differential equations to estimate vector fields that define the deformation between objects, and the surface that defines the segmentation of the objects as well. We also explore the utility of inequality constraints applied to variational problems in vision such as estimation of deformation fields in non-rigid registration and tracking. To solve inequality constrained vector field estimation problems, we apply tools from the Kuhn-Tucker theorem in optimization theory.

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**MS149**
**Using Nonlinear Model Predictive Control to Find Optimal Therapy Strategies to Modulate Inflammation**

Controlling inflammation has become a key focal point in the treatment of critically ill patients and the identification of proper biological targets and their specific manipulations is necessary. One means of achieving this end involves formulating a strategy for delivering therapies, in the correct amount, at the right time. A tool that can help determine this complex dose regimen is Nonlinear Model Predictive Control (NMPC). We apply NMPC in the setting of a 4-dimensional ordinary differential equations model of the acute inflammatory response to pathogen due to Reynolds and colleagues (JTB, 2006, v. 242). A patient population of 1000 randomly generated patients was considered. Of these virtual patients, 620 were recognized as being ill enough to receive treatment, as defined by levels of phagocytic cells exceeding a predetermined threshold. The algorithm identified individualized therapeutic strategies that enabled approximately 20-40% more patients to be successfully restored to homeostasis (damage reduced to baseline) as compared to other treatment strategies (e.g. non-individualized therapies or placebo). Current and future work will also be discussed.

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**MS149**
**Image Driven Parameter Identification**

The applied context of our problem is morphogenesis, which refers to the differentiation and growth of tissues and organs during embryonic development. In particular, biologists would like to know what controls the development of skin patterns in animals, for example, the stripes on a zebra, or the spots on butterfly wings. Due to the complexity of the biochemical reactions involved, the precise mechanisms involved in the development of skin patterns are still unknown. A possible mechanism that has been intensely studied, is the so called 'diffusion induced instability' of Turing, which relies on significant differences between diffusion rates of morphogens, and specific reaction kinetics. We present for the first time a general image driven methodology for parameter identification in Turing systems with wide applicability, using PDE constrained optimization techniques, and present numerical results for the well-known Gierer-Meinhardt and Schnakenberg reaction-

diffusion systems.

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**MS149**
**Inverse Problems in Biological Systems**

In this talk, we will look at a benchmark problem in parameter identification of biological systems. We will briefly look at current methods and then consider if iterated Tikhonov regularization can provide a better solution than current methods.

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**MS149**
**A Controllability Problem in Pattern Formation**

We study the controllability of the classic Gierer-Meinhardt reaction-diffusion system, used in pattern formation, by reducing it to the null-controllability of the linearized system via a fixed-point argument.

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**MS151**
**Parameter-preserving Model Reduction by an Interpolatory Balanced Truncation Approach**

Model reduction is common in simulation, control and optimization of complex dynamical systems. Quite often, these systems contain additional parameters, e.g., to allow for geometrical variation or modifications of boundary conditions. The preservation of the parameters in the reduced-order system is a highly desired task. Since usual approaches for model reduction of linear, time-invariant systems are not suitable, we derive a method which preserves the parameters $p = \{p_1, \ldots, p_d\}$ in a linear system

$$\dot{x}(t) = A(p)\, x(t) + B(p)\, u(t)$$

with parameter-dependent matrices $A(p) \in \mathbf{R^{n\times n}}$, $B(p) \in \mathbf{R^{n\times m}}$. The matrix $C \in \mathbf{R^{n\times p}}$ in the output equation

$$y(t) = C^T x(t)$$

is assumed to be constant. The parameter space is discretized by sparse grids; the resulting linear, time-invariant systems are reduced by the usual balanced truncation technique. The overall reduced-order system containing all parameters is obtained by interpolation.

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**MS151**
**Convergence and Shift Behavior for Arnoldi Methods**

Krylov subspaces form the foundation for a variety of popular algorithms, including moment-matching methods for the reduction of linear time-invariant dynamical systems. To reduce storage and algorithmic complexity, methods based on the Arnoldi process (full orthogonalization) can be restarted, whereby the starting vector is strategically filtered. We describe recent progress on the analysis of filters built on 'exact shifts' and the implications of these results for eigenvalue iterations and model reduction.

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**MS151**
**On Krylov Subspace Methods for Solving Matrix Equations**

Several model reduction techniques, in particular balanced truncation, require the solution of potentially very large matrix equations. This talk is concerned with Krylov subspace methods for solving matrix equations. Several techniques are proposed and analysed that aim at avoiding some of the drawbacks caused by the typically slow convergence of these methods.

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**MS151**
**On the Use of Distance to Nearest Uncontrollable System in the Actuator Placement Problem**

Designing feedback control systems involving fluid flows are challenging due to the complexity of simulating and/or estimating the flow properties. In this study we investigate the use of reduced order models based on the proper orthogonal decomposition (POD) for this problem. In particular, we consider numerical control system properties including distance to uncontrollability, distance to unstabilizability, and the conditioning of the associated low-dimensional algebraic Riccati equation to aid in the proper placement of actuators and sensors. This numerical study includes a control problem involving the two dimensional Navier-Stokes equations with the Boussinesq approximation simulating flow of air in a room.

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**MS152**
**Fluid-Structure Interactions at Microscopic Scales: Applications in Soft Matter Materials**

We shall discuss a multiscale modeling and simulation formalism for soft matter materials taking into account hydrodynamic interactions and thermal fluctuations. A specific motivation is the study of lipid bilayer membranes and polymer fluids taking into account microstructure degrees of freedom. The approach is based on the immersed boundary method, where hydrodynamic interactions of the

composite system are handled by an approximate treatment of the fluid-structure stresses. The microstructures (lipid molecules / polymers) are represented by Lagrangian degrees of freedom which are coupled to an Eulerian representation of the fluid, treated at the level of continuum mechanics. Thermal fluctuations are incorporated in the formalism by an appropriate stochastic forcing of the fluid-structure equations in accordance with the principles of statistical mechanics. The theoretical formalism presents a number of numerical challenges for temporal integration and spatial resolution which we shall address. This includes a time step integrator for the stiff stochastic dynamics and methods to handle adaptive spatial discretizations of the underlying stochastic partial differential equations. We shall discuss specific applications of the approach, including the study of lipid flow in bilayer membranes, the shear viscosity of polymer fluids, and the diffusivity of particles in complex fluids.

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**MS152**
**Vesicles and Red Blood Cells under Flow**

The flow behavior of cells and vesicles is important in many applications in biology and medicine. For example, the flow properties of blood in micro-vessels is determined by the rheological properties of the red blood cells. Furthermore, microfluidic devices have been developed recently, which allow the manipulation of small amounts of suspensions of particles or cells. While the membrane of vesicles just consist of a fluid lipid bilayer, red blood cells have a composite membrane which has in addition an anchored polymer network. This implies that the elastic properties of vesicles and red blood cells are very different. Due to the large length- and time-scale gap between the atomic and the mesoscopic domain in soft matter systems, several mesoscale simulation techniques have been developed in recent years to study their hydrodynamic behavior. We have investigated one of these techniques, multi-particle-collision dynamics, in some detail. In particular, it has been shown that the method properly describes hydrodynamic interactions at low Reynolds and high Schmidt numbers, if the parameters are chosen appropriately. This method has then be applied to study the dynamical bevavior of fluid vesicles and model red blood cells both in shear and capillary flows. Several types of dynamical behaviors as well as shape transformations occur as a function of shear rate (or flow velocity), membrane viscosity and internal viscosity, which will be discussed in some detail.

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**MS152**
**Active Microswimmers: From Individual Motion to Collective Structures**

Self propelling objects, such as microorganisms, displace by swimming in an embedding solvent. As a result of their displacements these microorganisms induce a solvent flow which perturbs the motion of nearby organisms. Such a coupling arises not only because of the effective modified friction force of close microorganisms, but also because it modifies their preferred displacement direction. I will describe, using a simple fluid mechanical model for organism displacement, how organism self-organization arises as a result of the coupling induced by the surrounding fluid.

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**MS152**
**Simulating the Microfluidics of Nonspherical Particulate Suspensions**

Colloidal dispersions with application in materials processing or biological assays often contain rod-like particles. In microfluidics applications, these suspensions often demonstrate qualitatively new flow phenomena. In this presentation, I will discuss two problems which exemplify these new phenomena as they have been studied via mean field theory, numerical simulation, and experiment. First, we examine the effect of Brownian motion on the stability of sedimenting fiber suspensions under an applied torque. In the second problem, we examine the microchannel pressure-driven flow of Brownian rodlike solutions.

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**MS153**
**A Sparse Composite Stochastic Collocation Method**

We present a new stochastic collocation method for solving elliptic PDEs on a domain $D \subset \mathbf{R^d}$ of the form

$$\begin{cases} \mathcal{L}(\sqcap) = \{ & \text{in D,} \\ mathcalB(u) = g & \text{on } \partial\text{D} \end{cases}$$

where the elliptic operator $\mathcal{L}$ and the source term $f$ are subject to inherent parameter uncertainties and $\mathcal{B}$ is a boundary operator. The uncertainty inputs are parameterized by means of a Karhunen-Loève expansion which is assumed to be finite. A hierarchic selection of finite element wavelet discretizations in physical space and a sequence of collocation operators in random parameter space, adapted to the stochastic regularity of the problem, are then used to derive a new formulation of a sparse collocation method which results in a considerable reduction of overall degrees of freedom. Numerical examples will then demonstrate the effectiveness of this new collocation approach.

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**MS153**
**Sensitivity Analysis via Smolyak Sparse Grids**

Smolyak sparse grids provide an efficient way of construct-

ing grid point sets in high dimensional spaces, compared to tensor grids which are impractical when the dimensionality is even modestly high. In term of stochastic computation, the Smolyak grids offer high accuracy at reasonble computational cost. In this talk, we discuss how Smolyak grids can be employed to conduct sensitivity analysis in an efficient manner. In particular, we adopt Sobol's decomposition to define sensitivity analysis and take advantage of the structure of the Lagrange interpolation polynomials of the sparse grids and develop a high-order algorithm.

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**MS153**

**Polynomial Chaos for Burgers' Equation with Stochastic Time-dependent Boundary Conditions**

Burgers equation with stochastic time-dependent boundary conditions is investigated using a polynomial chaos approach. The truncated problem is well-posed and converges to the analytical solution. Numerical discretization using summation by parts operators and weak boundary conditions are used to ensure stability. A characteristic analysis of the solution of the truncated system is presented and is compared to the analytical solution, thereby explaining qualitative differences such as occurrence of discontinuities in the truncated solution.

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**PP0**

**P4est: A Scalable Adaptive Mesh Library to Manage Forests of Octrees**

Adaptive mesh refinement (AMR) is essential for numerical solution of partial differential equations that describe many multiscale physical phenomena. Because of the complexity and large communication costs, the scalability of AMR has long been considered questionable. We present p4est, a new parallel mesh library from the ALPS project which enables scalable adaptivity on tens of thousands of cores not only on the unit cube but also on multiple connected octrees, covering arbitrary domains.

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**PP0**

**Metaheuristic Approaches for the Minimum Vertex Guard Problem on Simple Polygons**

The Minimum Vertex Guard problem on polygons is NP-hard. This computational complexity impedes methods which guarantee an optimal solution in the time available. In this situation different approaches are required, such as the use of metaheuristic techniques. In this paper we compare five approximation algorithms for that problem, one greedy, two metaheuristics (genetic algorithm and simulated annealing), and two hybrid metaheuristics. We conclude, through experimentation, that the best results are produced by hybrid metaheuristics algorithms.

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**PP0**

**Scalable Parallel 3d Ffts for Electronic Structure Codes**

First-principles methods based on Density Functional Theory (DFT) where the wavefunctions are expanded in plane waves (Fourier components) are the most widely used approach for electronic structure calculations in materials science. The scaling of this method to petaflop platforms depends critically on having an efficient parallel 3d FFT that minimizes communications and calculations. We present a comparison of different parallel implementations of a 3d FFT specifically designed for electronic structure calculations that scales to 10K processors on leading parallel supercomputer platforms. Work done in collaboration with Lin-Wang Wang, John Shalf and Manisha Gajbe.

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**PP0**

**Experimental Simulations of the Numerical Reuleaux Method for Lumbar Artificial Disc Implants IRC Determination**

The recently developed Numerical Reuleaux Method can be used to determine the IRC of artificial spine implants whose material structure is a pseudo-rigid body. The experimental simulations of this numerical algorithm have been carried out for artificial lumbar discs at the laboratory. The imaging data has been obtained from a RX-C-Arm machine as it is usual in the clinical practice. The imaging results and numerical simulations are presented in this scientific communication. The results of these experimental simulations agree to the theoretical numerical algorithm

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**PP0**

**DCT: Distributed Coupling Toolkit to Couple**

**Multi-Resolution Models**

Due the increase of the capabilities of the high performance computing, it is possible to formulate and handle more complex physical models. Enabling very high resolution model runs improves the physical phenomena approximation, and our ability to study interactions between different physical processes at different scales. The DCT is an user friendly coupling library that promotes a purely distributed computational environment, which can easily scale both the model complexity and number of processing elements.

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**PP0**

**Aliasing in Calculating Convolutions Using Random Fourier Series**

The goal of this project is to study the aliasing errors involved in performing convolutions in the stochastic setting using Fourier series, as well as the use of padding and the phase shift method to reduce this error. We present results in both the deterministic setting and the stochastic setting. This project was part of the NSF CSUMS program at NJIT for undergraduate research in computational science.

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**PP0**

**Terrain-Induced Rotors: Visualization in Three Dimensions**

Our poster will explore the three-dimensional particle trajectories as they are advected through terrain-induced rotors. We plan to display different visual interpretations of the rotors and particle movements, and will also offer an informative look on the nature of terrain-induced rotors and their effects on the atmosphere.

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**PP0**

**Algorithms for Recursively Rendering Parametric Curves**

Nonlinear dynamical systems are typically regulated by invariant manifolds, stable and unstable, that exhibit regions of erratic trajectories and very high curvature. We present a recursive algorithm for rendering parametric curves than can be applied to one-dimensional invariant manifolds. The method is based on adaptive evaluation of Catmull-Rom splines and improves on previous methods based on linear interpolation. We show numerically that the number of points needed to render the curve to a given accuracy is greatly reduced compared with previous methods.

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**PP0**

**A System of Bilinear Immersed Finite Elements (IFE)**

We first introduces a bilinear IFE space for elliptic interface problems. The partition can be independent of the interfaces. Our interpolation error estimates indicate that this nonconforming space has the optimal approximation capability. Then this space is implemented to Galerkin method, finite volume element method and discontinuous Galerkin method. Numerical examples and convergence analysis show that these methods have the optimal convergence rates. In a word, we are building a system of bilinear IFE.

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**PP0**

**Memory Use Prediction for Automatic Generation of Fused Linear Algebra Routines**

Combining multiple linear algebra routines through loop fusion usually reduces their overall memory access costs. Automatically creating fused routines reduces both programmer effort and application development time. Accurately predicting memory costs reduces the number of routines that must be created and tested in the automation process. In this poster, we show how to predict when loop fusion is effective and how to use that information to generate fused kernels quickly and automatically.

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**PP0**

**Sub-Nyquist Spectral Methods Via a Deterministic Sub-Linear Time Fourier Algorithm**

We investigate spectral methods on sub-Nyquist grids using a deterministic sub-linear time Fourier algorithm. This algorithm deterministically identifies $B$ of the most significant frequencies in the Fourier expansion of a given frequency-sparse signal of length $N \gg B$ and estimates their coefficients in poly(B, log(N)) time, using only a sub-linear number of samples. As proof-of-principle we study the 1-D heat equation with random forcing and compare our results with those based on randomized Fourier algorithms.

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**PP0**

**Modeling and Simulation of Vascular Beds with Recursive Convolution**

Accurate models and efficient implementations of vascular beds are necessary to estimate the pressure pulse in time and to understand the effects of changes in vascular properties, due to disease progression or compound intervention. We propose a recursive convolution method to simulate, in time, vascular-bed models specified by rational transfer functions. The efficiency of the proposed method is demonstrated by simulating a) outflow boundary conditions in a 1-D arterial tree model and b) vascular bed models connecting 1-D arterial and venous tree models.

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**PP0**

**Geoacoustic Inversion in the Ocean**

The behavior of the frequency content of an acoustic signal with time acts as a fingerprint of the propagation medium, when broadband signals with frequencies of a few hundred Hz propagate long distances in the ocean. This behavior is quantified via dispersion curves which can be estimated with time-frequency analysis. Arrival times of distinct modes are extracted from such an analysis and are used here with local and global inversion techniques to estimate environmental and source location parameters. Using probability distributions for the extracted arrival times, we also calculate uncertainty in our estimates.

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**PP0**

**Computation of the Density Distribution from Velocity Field Measurements in Sedimenting Suspensions**

A slowly sedimenting suspension with a variable density is considered. Using an eigenfunction expansion approach, measurements of the velocity field are used to obtain a numerical computation of the density. This inverse process will not however generate the entire density field given only the velocity field at one specific time. Using two measurements of the velocity field at close times we generate a complete view of the density distribution.

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**PP0**

**Generalized Fokker-Planck Approximation in Radiotherapy**

Particle processes in radiotherapy can be simulated by deterministic calculations coping with the problem of big dimensionality. The Fokker-Planck asymptotic approximation is one possibility to reduce the resultant high numerical effort. Its basis is the assumption that all scattering processes are highly forward-peaked. However, physical relevant kernels reveal a sufficient amount of large-angle scattering. Our main aim is to present a new Generalized Fokker-Planck theory, developed by Leakeas and Larsen to counteract this drawback, and demonstrate numerical experiments.

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**PP0**

**Simulating Bone Loss in Microgravity Using Mathematical Models of Bone Turnover**

This discussion presents the results of simulations of bone remodeling by numerical computation of the solution of a system of nonlinear ordinary differential equations that model the cellular dynamics. There are a number of proposed models in the literature that attempt to understand the causes of various bone diseases and possible therapies. We focus on one particular slightly modified model and concentrate on simulating the effects of microgravity. The first order system of nonlinear ODEs is typically solved numerically using Runge Kutta methods. The over goal of

developing a comprehensive model of the biological process of bone remodeling is also discussed as well as the modeling and numerical simulation challenges.

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**PP0**

**Data Reduction and Noise Removal Using the Maximum Noise Fraction and Hermite Splines**

Presented here is an adaptive noise filter applicable to data transformed by the maximum noise fraction (MNF). The adaptive filter exploits the properties of the MNF to alter filter size depending on estimated signal-to-noise ratios (SNRs) for each group of bands. Applying this adaptive filter to a high dimensional remote sensing image improved individual tree species identification accuracy by 10% in a 224-band image.

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**PP0**

**Integral Equation Methods for the Navier-Stokes Equations**

An integral equation formulation for the two dimensional incompressible Navier-Stokes equations is presented. This formulation is designed for solving equations arising from temporal discretizations of the stream-function formulation. Solving these equations requires use of standard potential theory as well as modern fast algorithms such as the Fast Multipole Method. The result is a highly efficent and accurate treatment of the underlying equations. Results concerning stability, complexity and accuracy will be presented.

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**PP0**

**How Expert Swing Dancers Exploit Physics**

We modeled a partnered spin in swing dance. In this movement, two dancers spin together around a common vertical axis. A theoretical model predicts the optimum spin pose for each couple through analysis of moment of inertia, torque and friction. To test the model, the motion of live dancers was captured using a 3D motion capture system. Finally, a physics based animation program, Maya, was used as a third note of comparison.

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**PP0**

**Rhea: Parallel Scalable Adaptive Mantle Convection**

Mantle convection is the principal control on the thermal and geological evolution of the Earth. To resolve highly localized phenomena for instance at faulted plate boundaries, adaptive meshes are essential. Rhea, which uses ALPS, combines dynamic mesh adaptation and scalable solvers for large-scale mantle convection simulations. We present results and scalings for end-to-end global mantle convection simulations with a finest local resolution of 1.5km that ran on up to 16,000 cores of the 580 Teraflops Teragrid system Ranger at TACC.

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**PP0**

**Aggregation in Multiscale Computations**

When analyzing systems with a large number of parameters, the dimension of the original system may present insurmountable difficulties for the analysis. It may then be convenient to reformulate the original system in terms of substantially fewer aggregated variables, or macrovariables. So-called iterative aggregation approach is considered in detail. It constructs an iterative process, at every step of which a macroproblem is solved that is simpler than the original problem because of its lower dimension. New classes of problems are presented where approximative and iterative aggregation is effective.

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**PP0**

**One Needle, Two Haystacks: Biomedical Simulations of Genetic Influences on Disease Biomarkers**

Genome wide scans produce data that can be assessed for its influence on disease or other phenotypic measurements. Various methods exist for discovering these relationships but, given the dimensionality of the problem, methodological comparisons are not simple. We use simulation to build

artificial data, based on real genetic data (to preserve the complex structure of real genetic data), and evaluate the performance of different discovery algorithms in detecting known probabilistic relationships between gene and phenotype.

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**PP0**

**A Mathematical Model of Early Brain Tumor Growth**

I present a mathematical model of blood vessel growth in glioblastoma multiforme, an aggressive form of brain cancer. The model incorporates the dynamics of growth factors relevant to the creation and destruction of the tumor vasculature. Quantitative and qualitative results of representative simulations are described.

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**PP0**

**Mangll: A Scalable Adaptive High-Order Discretization Library**

Adaptive mesh refinement and coarsening (AMR) is essential for numerical solution of partial differential equations (PDEs) that describe many multiscale physical problems. We present mangll, a high-order parallel discretization library from the ALPS project. The mangll library supports nodal elements on domains that are covered by a distributed hexahedral adaptive mesh with 2:1 split faces (such as provided by the p4est library). Implementation details and scalability results of mangll will be presented.

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**PP0**

**Simulation and Theoretical Analysis on Walking-Distance Introduced Queueing System**

We simulate and analyze pedestrian queueing system by using cellular automata. In our model the walking distance from the head of the queue to the service windows, which is not included in the queueing theory, is introduced. The most efficient type of queueing system is obtained from the queueing theory; however, we find that it changes according to the utilization of the queueing system and the ratio of service time to walking time.

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