IC1

On Dispersive Equations and Their Importance in Mathematics

Dispersive equations, like the Schrödinger equation for example, have been used to model several wave phenomena with the distinct property that if no boundary conditions are imposed then in time the wave spreads out spatially. In the last fifteen years this field has seen an incredible amount of new and sophisticated results proved with the aid of mathematics coming from different fields: Fourier analysis, differential and symplectic geometry, analytic number theory, and now also probability and a bit of dynamical systems. In this talk it is my intention to present few simple, but still representative examples in which one can see how these different kinds of mathematics are used in this context.

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IC2

On the Role of Error and Uncertainty in the Numerical Simulation of Complex Fluid Flows

The failure of numerical simulation to predict physical reality is often a direct consequence of the compounding effects of numerical error arising from finite-dimensional approximation and physical model uncertainty resulting from inexact knowledge and/or statistical representation. In this topical lecture, we briefly review systematic theories for quantifying numerical errors and restricted forms of model uncertainty occurring in simulations of fluid flow. A goal of this lecture is to elucidate both positive and negative aspects of applying these theories to practical fluid flow problems. Finite-element and finite-volume calculations of subsonic and hypersonic fluid flow are presented to contrast the differing roles of numerical error and model uncertainty for these problems.

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IC3

Communication Complexity of Algorithms

Algorithms have two kinds of costs: arithmetic and communication, which means either moving data between levels of a memory hierarchy (in the sequential case) or over a network connecting processors (in the parallel case). The costs of communication often dominate the cost of arithmetic. Thus, minimizing communication is often highly desirable. The main goal of this talk is to describe a general method for deriving upper and lower bounds on the amount of data moved (also known as bandwidth) for a very general class of algorithms, including most dense and sparse linear algebra algorithms. The method involves combinatorial analysis of computation graphs, in particular, of their expansion properties. This is joint work with Grey Ballard, James Demmel, and Oded Schwartz.

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IC4

Kinematics and Numerical Algebraic Geometry

Kinematics underlies applications ranging from the design and control of mechanical devices, especially robots, to the biomechanical modelling of human motion. The majority of kinematic problems can be formulated as systems of polynomial equations to be solved and so fall within the domain of algebraic geometry. While symbolic methods from computer algebra have a role to play, numerical methods such as polynomial continuation that make strong use of algebraic-geometric properties offer advantages in efficiency and parallelizability. Although these methods, collectively called Numerical Algebraic Geometry, are applicable wherever polynomials arise, e.g., chemistry, biology, statistics, and economics, this talk will concentrate on applications in mechanical engineering. A brief review of the main algorithms of the field will indicate their broad applicability.

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IC5

Cloaking and Transformation Optics

We describe recent theoretical and experimental progress on making objects invisible to detection by electromagnetic waves, acoustic waves and matter waves. For the case of electromagnetic waves, Maxwell's equations have transformation laws that allow for design of electromagnetic materials that steer light around a hidden region, returning it to its original path on the far side. Not only would observers be unaware of the contents of the hidden region, they would not even be aware that something was being hidden. The object, which would have no shadow, is said to be cloaked. We recount some of the history of the subject and discuss some of the mathematical issues involved.

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IC6

Algebraic Geometric Algorithms in Discrete Optimization

It is common knowledge that the understanding of the geometry of convex bodies has helped speed up algorithms in discrete optimization. For example, cutting planes and facet-description of polyhedra have been crucial in the success of branch-and-bound algorithms for mixed integer linear programming. Another example is how the ellipsoid method can be used to prove polynomiality results in combinatorial optimization. For the future, the importance of algebra and geometry in optimization is even greater since applications now demand non-linearity constraints together with discrete variables. In the past 5 years two beautiful algebraic geometric algorithms on polyhedra have been used to prove unexpected new results on the computation of integer programs with non-linearly objective functions. The first is Barvinok's algorithm for polytopes, and the second is Graver's bases method on polyhedral cones. I will describe these two algorithms and explain why we can now prove theorems that were beyond our reach before. I will also describe attempts to turn these two algorithms into practical computation, not just theoretical results. This is a nice story collecting results contained in several papers, joint work with various subsets of the following people: R. Hemmecke, M. Koeppe, S. Onn, U. Rothblum, and R. Weismantel.

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IC7

Scalable Tensor Factorizations with Incomplete Data

Incomplete data is ubiquitous in biomedical signal processing, network traffic analysis, bibliometrics, social network analysis, chemometrics, computer vision, communication networks, etc. We explain how factor analysis can identify the underlying latent structure even when significant portions of data are missing and the remainder is contaminated with noise. Though much of what we will say is also applicable to matrix factorizations, we focus on the CANDECOMP/PARAFAC (CP) tensor decomposition. We demonstrate that it is possible to factorize incomplete tensors that have an underlying low-rank structure. Further, there are approaches that can scale to sparse large-scale data, e.g., 1000 x 1000 x 1000 with 99.5% missing data. Real-world applicability is demonstrated in two examples: EEG (electroencephalogram) applications and network traffic data.

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IC8

Factorization-based Sparse Solvers and Preconditioners

Efficient solution of large-scale, ill-conditioned and highly-indefinite algebraic equations often relies on high quality preconditioners together with iterative solvers. Because of their robustness, factorization-based algorithms often play a significant role in developing scalable solvers. We present our recent work of using state-of-the-art sparse factorization techniques to build domain-decomposition type direct/iterative hybrid solvers and efficient incomplete factorization preconditioners. In addition to algorithmic principles, we also address many practical aspects that need to be taken into consideration in order to deliver high speed and robustness to the users of today's sophisticated high performance computers.

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IC9

Energy Efficiency in the Built Environment: Systems Approaches and Mathematical Challenges

Buildings consume nearly 40% of the world's energy, significantly more than either the transportation or industrial sectors. Any comprehensive plan to reduce atmospheric carbon must include actions to reduce energy consumption in the building sector. This talk will focus on the current understanding of the options available to reduce energy use in buildings and will highlight the role of mathematics and particularly computational science in delivering low energy buildings to the market in cost-effective ways. A systems approach to designing and operating low energy buildings will be described and the opportunities to develop and deploy methods for uncertainty quantification, dynamical systems and embedded systems will be highlighted.

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IC10

Semidefinite Programming: Algorithms and Applications

The last two decades have seen dramatic advances in the theory and practice of semidefinite programming (SDP), stimulated in part by the realization that SDP is an extremely powerful modeling tool. Applications of SDP include signal processing, relaxations of combinatorial and polynomial optimization problems, covariance matrix estimation, and sensor network localization. The first part of the talk will describe several applications, such as matrix completion, that have attracted recent interest in large scale SDP. The second part will focus on algorithms for SDP. First, we present interior-point methods (IPMs) for medium scale SDP, follow by inexact IPMs (with linear systems solved by iterative solvers) for large scale SDP and discuss their inherent limitations. Finally, we present recent algorithmic advances for large scale SDP and demonstrate that semismooth Newton-CG augmented Lagrangian methods can be very efficient.

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IP0

W. T. and Idalia Reid Prize in Mathematics Lecture: William T. and Idalia Reid: His Mathematics and Her Mathematical Family

The W. T. and Idelia Reid Prize in Mathematics was established in 1993 by SIAM and is funded by an endowment from the late Mrs. Idalia Reid to honor the memory of her husband Dr. W. T. Reid and his love of mathematics. Over time we often forget the people whose names are attached to the prizes that are periodically awarded for outstanding research or other contributions to our profession. Since I am the first of Professor Reid's students to be honored by this Prize, it is only fitting that I take this opportunity to review some of Dr. Reid's contributions to mathematics and Mrs. Reid's support of his mathematical colleagues and students.

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IP0

Julian Cole Prize Lecture: Mathematical Mod-

elling of Tissue Growth

Approaches to the continuum modelling of biological tissue growth will be described, with specific emphasis on (i) novel aspects of the resulting PDE formulations that arise from the biological contexts to which they are intended to apply and (ii) the role of singular-perturbation methods in elucidating model properties. The talk will focus on recent developments in the application of multiphase continuum-mechanics descriptions, particularly in describing the growth of engineered tissue within a porous scaffold.

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IP0

The AWM-SIAM Sonia Kovalevsky Lecture: Mixing It Up: Discrete and Continuous Optimal Control for Biological Models

This presentation will illustrate optimal control methods applied to several types of models, including a mixture of discrete and continuous features. The applications range from a discrete model for cardiopulmonary resuscitation to partial differential equation models for rabies in raccoons. Detailed results will be given for harvesting in a PDE fishery model that answer the question: Does a marine reserve occur when maximizing harvest yield?

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IP0

The John von Neumann Lecture - Algebra: From Linear to Non-Linear

This lecture will discuss recent applications of methods from abstract algebra in modeling and solving non-linear problems across the mathematical sciences. Techniques that are familiar from linear algebra have natural extensions in the non-linear world of algebraic geometry, whose recent advances are now transforming our thinking about problems arising in domains such as convex optimization, statistical inference and computational molecular biology.

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IP0

I.E. Block Community Lecture: The Geometry of Music

In my talk, I show how to translate the language of elementary music theory into that of contemporary geometry. It turns out that concepts such as "chord" and "chord type" are naturally represented by points in geometrical spaces known as "orbifolds." Understanding these spaces can help us to understand general constraints on musical style, as well as the inner workings of specific pieces. For example, we will see that Mozart, Chopin, and Schubert made very sophisticated use of a necklace of four-dimensional cubes representing four-note chords. The talk will be accessible to non-musicians and will exploit interactive 3D computer models that allow us to see and hear music simultaneously.

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IP1

Mathematical Challenges in Climate Change Science

Climate models solve the equations for the conservation of momentum, mass and energy in the atmosphere and oceans, the equations of state of air and for sea water, as well as equations for energy and water exchange with the land and cryosphere. This talk will present a brief review of the progress of climate modeling and will emphasis new challenges in projecting future climate change. Examples will include prediction of co-evolution of atmospheric CO2 and climate, carbon data assimilation, and chaotic transitions.

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IP2

Compressed Sensing: Survey and Applications

Compressed sensing is a very active area of recent research attracting researchers from approximation theory, information theory, harmonic analysis, statistics and signal processing. It has applications in areas ranging from speeding up medical imaging to enabling more ambitious deep-sky astronomy. In addition the topic combines a bit of paradox – seeming to show that traditional 'barriers' such as the Shannon-Nyquist sampling theorem don't apply – while also involving some pretty advanced ideas from high-dimensional geometry and even statistical physics. In my talk I will try to engage newcomers with a survey some of the excitement of this area, while also mentioning the sophisticated new ideas appearing almost daily. I will also try to bridge my talk to the associated minisymposia on Compressed Sensing.

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IP3

Closing the Loop: Computational Physics and the Industrial Design Process

Over the last two decades, improvements in computer hardware and the development of nearly linear scaling methods have brought a variety of large-scale calculations within practical reach. While these methods have had substantial impact in industry, a number of improvements are needed in order for these methods to be fully integrated into acoustic, electromagnetic, thermal and mechanical design environments. In this talk, we will describe the current state of the art, as well as some recent ideas that may lead to a new generation of fast solvers, enabling robust, automatic and geometrically flexible design by simulation.

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IP4

Transaction Costs

Stochastic calculus models for financial markets have played a fundamental role in finance in the past 30 years. The first application of these models is to determine the price of a derivative security by working out the strategy by which the security payoff can be replicated by trading in primary assets. The second application is to solve the stochastic control problem of maximizing the utility of investment. If there are no transaction costs for trading in assets, these problems have elegant solutions. This talk is discusses what can be done when transaction costs are present. The principal tool for analysis is a variational inequality version of the Hamilton-Jacobi-Bellman equation. Although this equation does not have an analytical solution, the initial terms in an asymptotic expansion of the solution can be obtained.

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IP5

Extension of Functions and Interpolation of Data

We discuss the problem of finding a C^m extension of a given real-valued function defined on an arbitrary given subset E of R^n. If E is infinite, then we ask how to decide whether an extension exists. If E is finite, then we ask for efficient algorithms to compute an extension with close-to-minimal C^m norm.

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JP1

The Dynamics of Obesity

The past two decades have seen a surge in the incidence of obesity in the developed world. Changes in body weight that can lead to obesity are known to result from imbalances between the energy derived from food and the energy expended to maintain life and perform physical work. However, quantifying this relationship has proved difficult. Here, I will show how simple concepts from dynamical systems can be used to provide a general quantitative description of how body weight will change over time. The model can then be used to answer open questions (and dispel some myths) regarding weight loss and gain and provide an explanation for the American obesity epidemic.

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CP1

Mathematical Model for the Behavior of Wildfires

Wildfires have been a long-standing problem in today's society. In this paper, we derive and solve a fluid dynamics model to study a specific type of wildfire, namely, a two dimensional flow around rising plume above a concentrated heat source modeling a fire line. This flow assumes a narrow plume of hot gas rising and entraining the surrounding air. The surrounding air is assumed to have constant density and is irrotational far from the fire line. Then the flow outside the plume is described by a Biot-Savart integral with jump conditions across the position of the plume. The plume model describes the unsteady evolution of the mass, momentum and energy inside the plume, with sources derived to model mixing in the style of Morton, et al. [1956]. The model is implemented in the same manner as structure-fluid interaction models [Alben and Shelley 2008], except that we include a sink term in the Biot-Savart integral to couple the entrainment into the plume to the potential flow around the plume. The results show that this model is capable of capturing a complicated interaction of the plume with the surrounding air. Morton, B. R., Taylor, Sir G. I., and Turner, J. S., Proc. Roy. Soc. London, A 234, 1-23 (1956). Alben, S. and Shelley, M. J., Phys. Rev. Letters, 100, 074301, (2008).

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CP1

Asymptotic Structure of Diffusion Flames at High Pressure with Soret Transport

Mathematical models of nonpremixed flames usually assume Fick's law applies to the molecular diffusivities. However, at elevated pressures, it is known that the Soret effects, i.e. mass transport via temperature gradients, become important. Moreover, at very high pressures, including supercritical conditions, Soret effects may become dominant. We investigate the asymptotic structure of diffusion flames with Soret mass transport. Our theory provides explicit expressions for flame temperature, location and extinction conditions in terms of physico-thermal parameters affecting combustion.

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CP1

Modes of Buckling of Viscous Fluid Threads

The 'coiling' of a thin thread of viscous fluid falling onto a surface is a familiar example of a buckling instability. Using an asymptotic 'slender thread' model embedded in a numerical continuation procedure, we show that the onset of coiling can occur in three distinct modes involving different balances of viscous forces, gravity, and inertia. We confirm these numerical predictions using laboratory experiments, which also reveal a previously unobserved 'rotatory folding' mode of finite-amplitude buckling. Hydrodynamic stability; turbulence (1704) Computational fluid dynamics (1707) Incompressible fluids (1701)

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CP1

Bifurcation and Chaos in Rotating Driven Cavity Flow

Numerical simulations of the incompressible Navier Stokes equations in a two-dimensional driven cavity are performed using high-order numerical methods. The effect of solid body rotation rate and Reynolds on flow stability is studied. The results show that the flow converged to a stationary state up to a certain rotation rate for a given Reynolds number. Above this critical value periodic oscillations indicative of Hopf bifurcation and eventually chaos are observed and analyzed.

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CP2

Weak-Material Approximations of Natural Boundary Conditions

The technique of Topology Optimization using the material distribution approach is increasingly used in the design of advanced mechanical components. This approach approximates natural boundary conditions at material interfaces by a fictitious-domain approach: a very weak material replaces regions of non-material ("void'). The energy-norm error associated with this approximation is shown to scale linearly with the weak-material density and with the norm of the boundary flux of a continuously extended solution to the original problem.

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CP2

The Effective Nonlinear Schrodinger Equation for Dark Spatial Plasmon-Polariton Solitons

We derive an effective Nonlinear Schrodinger Equation for propagation an optical dark spatial soliton at the subwavelength with surface plasmonic interaction. Starting with Maxwell's Equations we derive TM polarized type spatial solitons on a metal dielectric interface in which the dielectric is a Kerr medium that has self-defocusing. We numerically and theoretically study the beam dynamics of this nano-waveguide.

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CP2

Stochastic Simulation of Self-Organization in Materials

Ostwald ripening is the self-organization of components of two phase mixtures through a diffusive mechanism. This phenomenon has been modeled using stochastic partial differential equations derived from the underlying microphysics. In this talk, results from simulations using spectral schemes for stochastic partial differential equations are described and new results for improving the efficiency of such schemes will be described. These simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law.

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CP2

A Highly Effective Finite Difference Approach for Oscillatory Optical Beam Equations

This talk discusses a class of efficient and effective finite difference schemes for solving highly oscillated optical wave equations. To achieve the computational efficiency, mathematical transformations are used to map the complex model equations to coupled real differential equations. Then operator splitting strategies are introduced to decompose the acquired nonlinear differential equations. An Crank-Nicolson type discretization incorporates with parallel computation architectures is finally implemented under proper adaptations. The finite difference schemes constructed are numerically stable. Simulation experiments are given to illustrate our results, conclusions and expectations.

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CP2

Shocks Versus Kinks in a Discrete Model of Displacive Phase Transitions

We consider dynamics of phase boundaries in a bistable one-dimensional lattice with harmonic long-range interactions. Using Fourier transform and Wiener-Hopf technique, we construct traveling wave solutions that represent both subsonic phase boundaries (kinks) and intersonic ones (shocks). We derive the kinetic relation for kinks that provides a needed closure for the continuum theory. We show that the different structure of the roots of the dispersion relation in the case of shocks introduces an additional free parameter in these solutions, which thus do not require a kinetic relation on the macroscopic level. The case of ferromagnetic second-neighbor interactions is analyzed in detail. We show that the model parameters have a significant effect on the existence, structure and stability of the traveling waves, as well as their behavior near the sonic limit.

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CP2

Structure Preserving Tau Methods for Stochastic Chemical Systems

Tau leaping methods can efficiently simulate models of stiff stochastic chemical systems. However, most existing methods do not naturally preserve some chemical structures, such as integer-valued and nonnegative molecular population states. In this talk, we present structure preserving tau methods for simulating stochastic chemical systems. We illustrate the new methods through a number of biochemically motivated examples, and provide comparisons with existing implicit tau methods.

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CP3

Hopf Bifurcation of a Ratio-Dependent Predator Prey System with Time Delay

In this study, we consider a predator-prey system with time delay where the predator dynamics is logistic with the carrying capacity proportional to prey population. We study the impact of the time delay on the stability of the model and by choosing the delay time t as a bifurcation parameter, we show that Hopf bifurcation can occur as the delay time t passes some critical values. Using normal form theory and central manifold argument, we also establish the direction and the stability of Hopf bifurcation. Finally, we perform numerical simulations to support our theoretical results.

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CP3

Reconstructing Potentials from Zeros of One Eigenfunction

We study an inverse nodal problem, concerning the reconstruction of a potential of a Sturm-Liouville operator by using zeros of one eigenfunction as input. We propose three methods for the reconstruction, one of which is the Tikhonov regularization method. The explicit error bounds are calculated for all the three methods. In case there is measurement error, the Tikhonov regularization method is still convergent. The study is motivated by physical considerations.

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CP3

A Solution to An Ambarzumyan Problem on Trees

We consider the Neumann Sturm-Liouville problem defined on trees such that the ratios of lengths of edges are not necessarily rational. It is shown that the potential function of the operator must be zero if the spectrum is equal to that for zero potential. This extends a previous result which states that if the edgelengths of a tree are in rational ratio and the spectrum contains $\{(n\pi)^2\}$, then the potential function is zero. Our result gives a complete solution to this Ambarzumyan problem. For a proof, we compute approximated eigenvalues for zero potential by using a generalized pigeon hole argument, and make use of a recursive formula for characteristic functions.

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CP3

Existence of Solutions and Asymptotic Analysis of a Singularly Perturbed BVP

I will outline a proof of the existence of two solutions of a singularly perturbed BVP $\varepsilon y' + 2y' + e^y = 0,\ y(0) = 0,\ y(1) = 0$ for $0 < \varepsilon < 1/10$. Both the solutions have the same outer solution on $(0, 1]$, but different boundary behavior near $x = 0$. One of them is bounded, the other unbounded as $\varepsilon \to 0$. If time permits, I will briefly discuss a rigorous proof that the conjectured formal asymptotic expansion for the smaller solution is correct.

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CP3

Value Functions and Transversality Conditions for Infinite-Horizon Optimal Control Problems

The purpose of this paper is to establish the transversality condition at infinity as necessary and sufficient conditions for optimality in optimal control problems with an infinite horizon under nonsmoothness assumptions, dispens-

ing with any controllability condition on the velocity. We introduce the coercivity of the integrand, which plays a significant role in verifying the sufficiency of the transversality condition at infinity together with convexity assumptions. Consequently, it is possible to derive a new characterization of optimality in terms of the adjoint inclusions for the value function and the Hamiltonian, without using any transversality condition at infinity.

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CP3

The Inverse Nodal Problem and Ambarzumyan Problem for the p-Laplacian with Various Boundary Conditions

We study the issues of the reconstruction and stability of the inverse nodal problem for the one-dimentional p-Laplacain eigenvalue problem. A key step is the application of a modified Prufer substitution. Two associated Ambarzumyan problems are also solved. We consider the case of C^1 potentials with the Dirichlet boundary condition and extend to the case of integrable potentials with the periodic or anti-periodic boundary conditions.

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CP4

Effect Of Abrupt Expansion On Nanofluid Flow And Heat Transfer Characteristics: A Numerical Study

Using the standard k-e turbulence model, incompressible nanofluid flow is simulated. Effect of alumina volume concentration in water flow and heat transfer characteristics downstream of an axisymmetric sudden expansion is investigated. Assuming homogenous nanofluid, different alumina volume fractions in water, ranging from 0.01 to 0.05 are considered. The simulation revealed recirculation downstream of the expansion. Wall shear stress and heat transfer coefficient are shown to increase linearly with increasing alumina volume fraction, up to 14% for alumina volume fraction of 0.05. It is shown that the boundary layer reattachment length is insensitive to alumina volume fraction under the assumptions invoked.

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CP4

A Mixed Implicit-Explicit Multirate Numerical Scheme for Time-Dependent Equations

We develop a multirate time integration method for systems of time-dependent equations that present two significantly different scales within the model. We use an iteration scheme to decouple the two time scales. At each iteration, we use an implicit Galerkin method to solve for the fast scale variable and an explicit method to solve for the slow variable. The error equation consists of a computable leading order term and a provably higher order expression.

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CP4

Domain Decomposition Methods for Coupled Stokes-Darcy Model

The Stokes-Darcy model arises in many applications such as surface water flows, groundwater flows in karst aquifers, and petroleum extraction. It has higher fidelity than either the Darcy or Stokes systems on their own. However, coupling the two constituent models leads to a very complex system. This presentation discusses the domain decomposition methods for solving the coupled Stokes-Darcy system. Convergence of these algorithms is demonstrated and the results of computational experiments are presented to illustrate their features.

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CP4

Solving High Speed Flow Problems with An Improved Version of Ice.

The Implicit Continuous-fluid Eulerian(ICE), a semi-implicit finite-volume solver, is used for simulating problems in multiphase flow which span a wide area of science and engineering. ICE is utilized by the C-SAFE code Uintah at the University of Utah to simulate explosions, fires and other fluid and fluid-structure interaction phenomena. The implementation of ICE used in Uintah is given in many papers by Kashiwa at Los Alamos and extended to solve multifield cases by Harman at Utah. In its original form the ICE algorithm does not perform as well as the best current methods for compressible flow problems. An improved version of ICE method using limiters is discussed and the obtained numerical results for several test problems are shown.

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CP4

A Particle-in-Cell Method with Remapping and

Local Mesh Refinement for Plasma Physics

The Vlasov-Poisson equation describes the kinetic behavior of a collisionless plasma. We present an accurate and stable particle-in-cell based algorithm for solving the Vlasov-Poisson equation. The method overcomes the numerical noise inherent in the usual particle-in-cell methods by periodically remapping the distribution function on a hierarchical of regularized grids. Positivity can be preserved through the novel use of a limiter. The method has successfully been applied to a set of one-dimensional problems, e.g., strong Landau damping, two stream instability. Second order accuracy is observed over short times. Over long times, the test problems gradually evolve into a weakly collisional domain. There, filamentation in velocity space develops which leads to instability and loss of accuracy. We solve this issue by introducing a collisional term to the Vlasov-Poisson equation. The collision equation is solved on the remapping grids periodically, and coupled to the system using operator splitting. Second order accuracy is obtained for the coupled system.

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CP4

A Lagrangian Vortex Method for Barotropic Vorticity Equation on a Rotating Sphere

We present a Lagrangian vortex method for the barotropic vorticity equation on a rotating sphere. The method tracks the flow map and absolute vorticity using Lagrangian particles and panels. The velocity is computed from the Biot-Savart integral on the sphere. An adaptive refinement strategy is implemented to resolve small-scale features and a treecode is used for efficient computation. Results are presented for Rossby-Haurwitz waves and vortex interactions.

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CP5

Asymptotics and Computation on Brownian Motion Escape

This talk will focus on asymptotics of partial differential equations arising from motion within a sphere with a small gate for escape. Computational methods will be used to compare via statistical analysis with the theoretical results to determine whether they are consistent, and also to explore the limitations of the theory.

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CP5

Predictability in Stochastic Dynamical Systems

This talk presents sensitivity and predictability analysis of stochastic reaction networks. Polynomial chaos expansions are used to efficiently perform non-intrusive parametric uncertainty propagation in the presence of intrinsic noise. The effects of strong nonlinearities and bimodalities in the forward model are relieved with an adaptive, dimension-specific domain decomposition technique. The curse of dimensionality is addressed using sparse quadrature methods for orthogonal projections.

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CP5

On the Maximum Entropy Solution to PDE-Based Inverse Problems

We present a novel approach, based on the principle of maximum entropy, to statistical inverse problems constrained by partial differential equations (PDEs). Indirectly observable parameters are estimated by a probability distribution that best represents our current state of knowledge and does not impose additional synthetic constraints. Uncertainty is quantified naturally by information entropy, a by-product of our inversion method. Results are compared to the standard Bayesian approach for a thermal conduction problem.

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CP5

Multiscale Methods for Statistical Inference in Elliptic Problems

Estimating the coefficients of an elliptic or parabolic PDE from observations of the solution is typically an ill-posed problem. Finite data resolution and the smoothing character of the forward operator limit one's ability to recover

fine-scale information. We use the multiscale finite element method (MsFEM) to formulate a low-dimensional and computationally efficient inference problem in this context. A fully Bayesian treatment of the problem conditions both small-scale and large-scale variability in the coefficients on available data.

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CP5

A Multi-Scale Random Basis Method for Stochastic PDEs

Uncertainty quantification is important in the field of engineering and applied mathematics. In this talk I will introduce a multi-scale random basis method for elliptic PDE with random coefficients. We first derive the multi-scale random basis offline based on the Karhunen-Loève decomposition using Monte-Carlo simulations for one particular non-zero force term. Then we use the multi-scale random basis to solve the elliptic PDE for a general force term. One important advantage of this method is that only very small number of random bases is required to accurately represent the stochastic solution, thus providing significant saving in the on-line computational effort compared with existing methods. Numerical results will be provided to demonstrate the effectiveness of the method.

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CP5

A Stochastic Heterogeneous Multiscale Method for Porous Media Flow

A stochastic heterogeneous multiscale method is introduced for modeling flows in heterogeneous media. To account for the high stochastic dimensionality of the permeability field, we employ the recently developed stochastic high dimensional model representation (HDMR) technique for the solution of stochastic PDEs. HDMR decomposes the original high-dimensional problem into several lower dimensional sub-problems which are efficiently solved using adaptive sparse grid collocation. The methodology is demonstrated through a number of benchmark examples of flows in porous media.

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CP5

American Option Pricing Models and Obstacle Problems

We first give a brief overview of American option pricing models and numerical methods. We treat American option models as a special class of obstacle problems. Finite element formulation is introduced together with error analysis of numerical solutions. Some interesting arbitrage properties about sensitivity of the option price to the payoff function are proved. We also give a criterion for the convergence of numerical free boundaries (optimal exercise boundaries) under mesh refinement. Some future research plans will be discussed.

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CP6

The Two-Machine Flowshop Scheduling Problem to Minimize Maximum Lateness

This study addresses a two-machine flowshop scheduling problem to minimize maximum lateness where processing times are random variables with lower and upper bounds. Given that the problem is NP-hard, we propose several algorithms and heuristics. The proposed algorithms and heuristics are compared through randomly generated data. The computational analysis has shown that one of the proposed heuristics performs very well with an overall average percentage error of less than one.

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CP6

Matrix Splitting Method Combined with the Gradient Projection Method for Support Vector Machines

We propose the matrix splitting method combined with the gradient projection method can be applied for the quadratic programming problem with a single linear equality constraint and box constraints arising in training support vector machines. The support vector machine problem has a dense Hessian matrix. The matrix splitting algorithm transforms the problem into a sequence of approximate subproblems which have a diagonal Hessian matrix and can be solved by the efficient pegging algorithm. The gradient projection method is combined with the matrix splitting method to reduce its sensitiveness. Some techniques for calculating the stepsize and non-monotone line search are applied for the proposed method to compare their performances. In addition, we use the incomplete Cholesky decomposition method for large scale problems. Our experimental results show the viability of the proposed algorithm.

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CP6

On the Extremal Problem of Polya

The notion of transfinite diameter of planar sets was introduced by M. Fekete around 1920s. This concept plays an important role in the classical complex analysis and is related to other well-known concepts such as the logarithmic capacity and Chebyshev polynomials. The transfinite diameter of a compact set in the complex plain is the limit of n-diameters of the set. For each $n \geq 3$, the n-diameter $d_n(E)$ of E is given by

$$d_n(E) = max \left\{ \prod_{1 \leq i < j \leq n} /z_i - z_j/^{\frac{2}{n(n-1)}} \right\}, \qquad (1)$$

where the maximum is taken over all n-tuples $\{z_1, z_2, \cdots, z_n\}$ of points in E.

The following is the extremal problem of G. Polya: among all n-tuples $E = \{z_1, z_2, \cdots, z_n\}$ with $|z_i| \leq 1$, find one with the largest n-diameter. The solution of this problem, attributed to Polya, is given below.

$$d_n(E) \leq n^{\frac{1}{n-1}} \qquad (2)$$

and the equality holds for n-tuples of equally spaced points on the boundary of D. While investigating the transfinite diameter of sets of constant width, Prof. Zair Ibragimov was led to the following weaker version of Polya's problem: among all n-tuples $E = \{z_1, z_2, \cdots, z_n\}$ with $|z_i - z_j| \leq 2$, find one with the largest n-diameter. He conjectured that the extremal configuration will also be the vertices of a regular n-gon, at least when n is odd. In this paper, I will present my solution of Ibragimov's problem for the case $n = 5$ and approach for $n = 7$. I will also discuss why other cases can not be proved using the same method as for $n = 5$.

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CP6

A Binary Tree Based Search Algorithm for Global Optimization

We describe a binary tree based search method for solving global optimization problems in the framework of a recently developed memoryless interval-based optimization method. It attempts to improve the reliability of the memoryless algorithm while sacrificing little both in memory space usage and in overall speed of convergence. A binary tree data structure is introduced as a means of memory that would guide the algorithm to locate a new approximate solution, while the overall algorithm employs the memoryless algorithm iteratively.

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CP6

An Inexact Trust-Region Based SQP Method for Nonlinear Programming Problems with Dense Constraint Jacobians

We present a trust-region based SQP algorithm for the solution of optimization problems with general non-linear constrained problems. Compared to traditional SQP algorithms, this algorithm does not require the exact evaluation of constraint Jacobian in each optimization step but uses an approximation of the first-order derivative information. Hence the proposed algorithm is well suited to solve optimization problems where the constraint Jacobian is dense i.e. the time required for the computation of the Jacobian and its factorization dominates the overall optimization process. The quality of the approximated constraint Jacobian can be adjusted by verifying two conditions that measure the inexactness of the null space representation (Walther, 2008) which can be easily verified during the optimization process. The performance of the algorithm is tested on a set of CUTE problems and dynamic optimization problems resulting from periodic adsorption processes whose constraint Jacobian is dense.

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CP6

Image Space Analysis and Scalarization for Optimization of Multifunctions

Using a new method based on generalized sections of feasible sets, we obtain optimality conditions for vector optimization of objective multifunction with multifunction constraints. In particular, necessary and sufficient conditions for scalarization of ε-optimization for multifunctions are deduced.

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CP7

Mortar Mixed Finite Element Method for Curved Domains

We present a mortaring (or a domain decomposition) method for the Darcy problem that can handle curved domains. The meshes are allowed to be non-matching over the subdomain interfaces and the continuity is enforced weakly via mortars, i.e. Lagrange multipliers. We show error estimates and confirm the results with numerical examples.

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CP7

Numerical Solution of Nonlinear Two-Dimensional Parabolic Partial Differential Equations by Branching Stochastic Processes

A new parallel numerical algorithm based on generating suitable *random trees* by Monte Carlo has been developed for solving nonlinear parabolic partial differential equations. While classical techniques based on a deterministic *domain decomposition* exhibits strong limitations, probabilistic methods are capable of exploit massively parallel architectures since the problem can be fully decoupled. New examples of nonlinear equations have been run on a high performance supercomputer, showing a remarkable scalability and performance.

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CP7

Multiple Scattering from Complexly Shaped Coated Obstacles

A numerical technique consisting of the Helmholtz equation in curvilinear coordinates coupled with an almost exact Dirichlet-to-Neumann boundary condition is applied to multiple scattering from coated obstacles of arbitrary shape. Novel elliptic grids conforming to complex geometrical configurations of several two-dimensional coated obstacles are constructed and approximations of the scattered field supported by them are obtained. The numerical results illustrate the ability of the proposed technique to deal with heterogeneous media.

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CP7

Strong Superconvergence of Finite Element Methods for Linear Parabolic Problems

We study the strong superconvergence of a semi-discrete finite element scheme for linear parabolic problems on $Q = \Omega \times (0, T]$, where Ω is a bounded domain in $\mathcal{R}^{\lceil}(\lceil \leq \triangle)$ with piecewise smooth boundary. We establish the global two order superconvergence results for the error between the approximate solution and the Ritz projection of the exact solution of our model problem in $W^{1,p}(\Omega)$ and $L_p(Q)$ with $2 \leq p < \infty$ and the almost two order superconvergence in $W^{1,\infty}(\Omega)$ and $L_\infty(Q)$. Results of the $p = \infty$ case are also included in two space dimensions ($d = 1$ or 2). By applying the interpolated postprocessing technique, similar results are also obtained on the error between the interpolation of the approximate solution and the exact solution.

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CP7

Numerical Methods for Elliptic and Parabolic Equations in Perforated Domains

Let ϵ denote the size ratio of the holes of some perforated domain to the whole domain. As ϵ closes to 0, a direct numerical simulation of the solutions of elliptic equations in perforated domains can be very expensive. It is known that the elliptic solutions approach a solution of some homogenized equation when ϵ is very small. It is reasonable to expect that the numerical approximation of the solution of the homogenized equation is a good approximation for the elliptic solutions in perforated domains when ϵ is small enough. We use standard numerical methods to obtain the approximation for the homogenized elliptic solution and to derive the L^∞ estimate, L^2 gradient estimate, and Lipschitz estimate for the difference between the exact elliptic solutions and the numerical approximation of the homogenized solution. Counterpart results for parabolic equations are also obtained.

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CP7

New Immersed Finite Element Methods For Planar Elasticity Interface Problem

We will discuss immersed finite element (IFE) methods for solving the planar elasticity interface problems with Cartesian meshes. The new IFE functions are formed on Cartesian meshes independent of the interface between different elastic materials. Some basic properties of the IFE functions will be presented including the optimal approximation capability of these IFE functions spaces. Furthermore, numerical examples indicate that these IFE methods converge optimally in both L^2 and semi-H^1 norms.

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CP8

Improved Bounds on Restricted Isometry Constants for Gaussian Matrices

The Restricted Isometry Constants (RIC) of a matrix A measures how close to an isometry is the action of A on vectors with few nonzero entries, measured in the ℓ^2 norm. Specifically, the upper and lower RIC of a matrix A of size $n \times N$ is the maximum and the minimum deviation from unity (one) of the largest and smallest, respectively, square of singular values of all $\binom{N}{k}$ matrices formed by taking k columns from A. Calculation of the RIC is intractable for most matrices due to its combinatorial nature; however, many random matrices typically have bounded RIC in some range of problem sizes (k, n, N). We provide the best known bound on the RIC for Gaussian matrices, which is also the smallest known bound on the RIC for any large rectangular matrix. Improvements over prior bounds are achieved by exploiting similarity of singular values for matrices which share a substantial number of columns.

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CP8

A Mathematical Model of Communications Networks

The behavior of a communication network can be modeled at the node/link scale as traffic units flowing along the links connected by nodes. We present an approach to packet flow that derives the node/link network model and connects it to a fluid-like model of traffic flow. The discrete node/link model describes packet queuing and the flow of packets from spatial point to spatial point. The model assumes that packets reside in buffers at each node, and are identified by their destination and the length of time they have resided in the buffer. An algorithm was created for packets to exit the buffer at each node according to their age ("first in, first out") and travel to the next node along a predetermined path to their destination. This algorithm calculates the rate at which packets distribute themselves to the next link in the route to their destination, assumes a source of packets originating at the node, and subtracts packets arriving at their destination. A continuum model is derived from this discrete flow model by associating each node with a spatial area defined by Voronoi polygons. The association with spatial areas leads to a flow continuity equation. The continuity equation describes the density of packets as a function of time and space, so that we are able to predict changes in global flow patterns on a macroscopic scale due to aberrant flow behavior, such as outages or heavy traffic. Exact (non-classical) solutions are derived for one dimensional flows using the method of characteristics. These solutions show that if a combination of the packet sources and network flow saturate the network flow capacity, the packet density grows at the nearest upstream node. When the source strength is reduced, or when flow is restored, the buffered packets flow at capacity until the density has been reduced. Multiple sources and destinations and multidimensional effects are discussed

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CP8

Modeling Adaptive Protocols for Wireless Sensor Networks Using Slime Mold

We present a new protocol for wireless sensor networks (WSNs) based on models of network self-assembly in *Physarum polycephalum*, a true slime mold. Slime mold assembles and modifies networks of tubes to distribute resources throughout its cell body. This system offers an elegant solution to resource allocation problems similar to extracting data from WSNs. We present modeling, analysis and simulation of this protocol for WSNs based on models of *Physarum polycephalum*.

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CP8

An Iterative Thresholding Algorithm Using Enhanced Sparsity

In this paper we propose a variation of the iterative soft-thresholding algorithm that is used to find sparse (approximate) solutions to the equation $Ax = b$. In this variation, the sparsity of the iterate vector x_n is used to redefine the regularizing penalty function. Minimization of the newly defined penalty function, then leads to the next iterate. Numerical data showing effectiveness of this approach will be presented as well.

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CP9

A-Posteriori Estimator for Parabolic Coupled Systems of Pdes

We present an extension of recent results by [Bernardi et al] and [Verfurth] on residual a-posteriori estimators for scalar parabolic PDEs. Our results concern multilevel discretization of parabolic systems in which each component can be computed on a different grid. We analyze contribution of each term and show convergence results. The estimator is robust i.e. the efficiency index remains essentially constant when the coefficients of the system vary even by several orders of magnitude.

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CP9

Preconditioning for Implicit Ocean Models

One challenge in ocean modeling is the spin-up problem, which requires integrations over centuries of time. Using implicit methods to take large timesteps requires effective preconditioners. We examine thin stratified fluid problems as modeled by the Parallel Ocean Program(POP), considering multilevel preconditioners for the velocity-salinity-temperature subproblem and block preconditioners fully coupled system. We present theoretical results to guide the choice of preconditioners as well as numerical results illustrating the effect of those choices in practice.

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CP9

ADI As Preconditioner for Krylov Subspace Methods in Serial and Parallel

The alternating directions implicit (ADI) method is a classical iterative method for numerically solving linear systems arising from discretizations of partial differential equations. We use ADI as a preconditioner for Krylov subspace methods for a linear system from a finite difference approximation of an elliptic test problem in three dimensions. The method is attractive because it allows highly efficient matrix-free implementations both in serial Matlab and in parallel C with MPI.

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CP9

Adaptive Finite Element Method for Elliptic Equations over Hierarchical T-Meshes

Isogeometric analysis based on NURBS (Non-Uniform Rational B-Splines) as basis functions preserves the exact geometry but suffers from the inconvenience of a purely local refinement. In this paper, we use the so called polynomial splines over hierarchical T-meshes (PHT-splines) to construct basis functions which share the similar properties as B-splines, and allow us to overcome the difficulty of refining a mesh locally. We present a residual-based a posteriori error estimate for the finite element discretization of elliptic equations using PHT-splines basis functions. Then numerical experiments are presented to verify the theoretical results and demonstrate the robustness of the error estimate.

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CP9

Robust Multigrid Preconditioners for the High-Contrast Diffusion and Biharmonic-Plate Equations

We study finite volume discretization of high-contrast diffusion equation and HCT and Morley discretizations of high-contrast plate equation. We construct preconditioners that are robust with respect to the magnitude of the coefficient contrast and mesh size simultaneously. For that, we prove robustness of the preconditioner proposed by Aksoylu et al. (2008) by extending the devised singular perturbation analysis to the above discretizations leading to a same family of preconditioners used for different PDEs and discretizations.

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CP10

New Upper Bounds on the Complexity of $\backslash\surd$-Complete Algorithms

In this talk we derive some new upper bounds on the complexity of algorithms which can solve $\mathcal{NP}$-Complete problems. Also upper bounds on the complexity of algorithms which have a high likelihood of solving $\mathcal{NP}$-Complete problems within the given complexity bounds will be discussed. Emphasis will be placed on one or two $\mathcal{NP}$-Complete problems.

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CP10

Production Lot Sizing with a Secondary Outsourc-

ing Facility

An extended Economic Production Quantity (EPQ) model is investigated in this paper where a fixed lot sizing policy is implemented to reduce the complexity of production planning and inventory control, and outsourcing with a secondary facility is used to supplement the lot sizing policy and to cope with the random demand. The considered cost includes: set up cost for the batch production, inventory carrying cost, backorder cost when the demand cannot be met during the production period, and outsourcing cost when the total demand is greater than the lot size in one production cycle. Under some mild conditions, the expected cost per unit time can be shown to be convex with respect to the lot size. The average cost reduction of the proposed model is 57.5%, when compared with that of the classical lot sizing policy. Outsourcing in the production lot sizing policy contributes to a significant portion of this cost savings when the mean demand rate is high. The numerical results also demonstrate that randomness of demand has significant impact on the lot sizing policy.

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CP10

Static Vertex Reordering Schemes for Local Mesh Quality Improvement

Vertex reordering can be performed within the context of local mesh quality improvement with the goal of decreasing the amount of time required for the mesh optimization. In this talk, we investigate various static vertex reordering schemes, based on mesh quality and the performance of the optimization algorithm, and the trade-offs between ordering and overall performance of the optimization algorithm. The study uses the Laplace smoother within the Mesquite package to optimize hexahedral meshes.

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CP10

Minimizing Weighted Quadratic Functions of Job Lateness in the Single Machine Scheduling System with Inserted Idle Time

This paper studies the problem of finding optimal schedules that minimize the weighted sum of some quadratic functions of job lateness on a single processor where an idle time is inserted before the processing of the first job begins. We introduce a novel exact two-stage algorithm for this NP-hard problem based on a precedence relation structure among adjacent jobs. Our computational results demonstrate that the algorithm can solve very large problem instances quickly on a PC.

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CP10

A Polynomial Arc-Search Path-Following Algorithm for Linear Programming

A simple analytic arc is proposed to approximate the central path of the linear programming. A primal-dual path-following interior-point algorithm is developed to search the optimal solution along the analytic curve. The algorithm is proved to be polynomial with complexity bound $O(n^{\frac{1}{2}} \log(1/\epsilon))$. Numerical test is conducted for problems in Netlib. The result shows that the new algorithm is promising compared to Matlab optimization toolbox `linprog` which implements the state-of-art Mehrotra's predictor-corrector algorithm.

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CP11

Nonlinear Asymptotic Stability in the Semi-Strong Pulse Regime for the Gierer-Meinhardt Equation with N-Pulse Positions

This paper shows the nonlinear asymptotic stability of an N-pulse solution to the Gierer-Meinhardt equation. Using semigroup and resolvent estimates, we are able to prove stability with renormalization group methods. In the semi-strong limit the localized activator pulses interact strongly through the slowly varying inhibitor. The interaction causes pulse amplitudes and speeds to change as the pulse separation evolves. In addition the point spectrum of the associated linearized operator evolves with the pulse dynamics.

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CP11

Nonsmooth Systems and Their Application

For many years, nonsmooth systems have been used as simplifications for certain types of smooth systems. In this talk we will show how this approach can lead to significant differences between solutions of both systems. We will illustrate the talk using the example of a genetic regulatory network.

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CP11

Traveling Waves Driven by Spatio-Temporally Varying Stimuli in Neural Field Equations

We examine the existence of traveling waves for continuum neuronal networks modeled by integro-differential equations. For a scalar field model with a general firing rate function and spatio-temporally varying stimulus, we show stimulus-locked fronts exist for a certain interval of stimulus speeds. We also add a slow adaptation equation and obtain a formula, involving an adjoint solution, for stimulus speeds that induce locked pulses and perform a singular perturbation analysis to approximate the adjoint.

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CP11

On the Stability of An Operator-Difference Scheme for Non-Linear Hyperbolic Differential Equation

We study the stability of second-order of accuracy difference scheme for the nonlinear hyperbolic equation $u''(t) + A(t)u(t) = f(t, u, u')$ $(0 \leq t \leq T), u(0) = \varphi, u'(0) = \psi$ in a Hilbert space H with the self-adjoint positive-definite operator $A(t)$ with the domain of $D(A(t))$. A new second-order of accuracy difference scheme with operator coefficient in a Hilbert space for the approximate solution of the initial-value problem is contracted. The stability estimates for the solution of this difference scheme are established.

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CP11

Mixed-Mode Oscillations in the Koper Model

Mixed-mode oscillations (MMOs) appear in a wide variety of applied dynamical systems arising in chemistry, biology and physics. The model investigated by Koper in 1995 provides an illustration how fast-slow system mechanisms can explain the complicated MMO patterns. We shall illustrate the techniques required for the analysis which include analytical as well as numerical ideas. An outlook on a possible general classification of MMOs will be given as well.

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CP11

Parallel Time Integration for a Membrane Problem

A Ratio-based Parallel Time Integration method is applied to a membrane second order initial value problem, given by $y^{'} - b|y^{'}|^{q-1}y^{'} + |y|^{p-1}y = 0$, where $p \leq q \leq 2p/(p+1)$. The solution $y(t)$ exhibits an oscillatory behavior and blows-up as t tends to infinity. After transforming the initial value problem into a first order system of ordinary differential equations, we use a method that automatically generates time-slices and rescales the time variable over every slice. Theoretically, in the case when $q = 2p/(p+1)$, such method leads to invariance with respect to the time slices in the sense that the computation of $y(t)$ is reduced to its finding over one slice. Whereas in the case when $p \leq q < 2p/(p+1)$, the method yields asymptotic similarity to a limit model, in the sense that the the rescaled systems admit a limit system. In both cases, this leads to an interesting Ratio based Parallel Time Integration algorithm - RaPTI. Its implementation on a cluster of 2 to 8 processors proves to be extremely efficient (decreasing execution time when increasing the number of processors).

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CP12

Shift-Invert Arnoldi Approximation to the Toeplitz Matrix Exponential

The shift-invert Arnoldi method is employed to generate an orthonormal basis from the Krylov subspace corresponding to a real Toeplitz matrix and an initial vector. The vectors and recurrence coefficients produced by this method are exploited to approximate the Toeplitz matrix exponential. Toeplitz matrix inversion formula and rapid Toeplitz matrix-vector multiplications are utilized to lower the computational costs. For convergence analysis, a sufficient condition is established to guarantee that the error bound is independent of the norm of the matrix. Numerical results are given to demonstrate the efficiency of the method.

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CP12

Inexact Newton and Krylov Methods for Riccati Equations

We explore the use of Inexact Newton methods to obtain a low-rank solution of the Continuous-time algebraic Riccati equation. That is, we are looking for $X_* = YY^T$, with $Y \in \mathbf{R}^{n\times p}$, $p \ll n$, such that $F(X_*) = 0$ where $F(X) = AX + AX^T - XBB^TXA + C^TC$, $A \in \mathbf{R}^{n\times n}, B \in \mathbf{R}^{n\times m}, C \in \mathbf{R}^{q\times n}$, and $m, q \ll n$. The standard formulation of the Newton method for this problem implies the solution of a (different) Lyapunov equation at each iteration. We use a Krylov projection method to find an approximate low-rank solution of this Lyapunov equation. As is well known,the accuracy of these approximations do not need to be too precise at first, but need to improve as the (outer) Newton method proceeds. We also explore the use of some recycling strategies to reduce the computational cost.

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CP12

The Iterative Solution of General Finite Linear Systems Via Flexible New Dual Variational Principles

These principles provide promising new approaches to numerically solving general systems of linear equations and/or linear inequalities – including general linear optimization problems. The resulting methodologies require only the numerical computation of a critical solution for an unconstrained objective function – carefully chosen for each individual problem from an infinite number of candidate functions, with the intent of employing parallel processors and/or exploiting any special system structure (such as sparsity). This infinite flexibility makes these new iterative solution methodologies competitive with, as well as much more general than, the previously developed iterative solution methodologies for solving large-scale linear systems – including both the conjugate-gradient method for symmetric positive-definite systems of linear equations and the interior-point methodologies for linear optimization. Finally, this presentation provides an introduction to the basic ideas and fundamental theory of generalized geometric programming, within the familiar context of elementary linear algebra, using only elementary convexity theory and multi-variable differential calculus.

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CP12

Fast Exponential Time Integration for Pricing Options in Jump-Diffusion Models

We consider pricing options in jump-diffusion models which require solving partial integro-differential equations. Discretizing by the central spatial finite difference scheme leads to linear systems of ordinary differential equations with Toeplitz structure. A fast exponential time integration scheme, where the shift-invert Arnoldi method is employed for the Toeplitz matrix exponential, is proposed to approximate the solutions of those systems. Numerical results are given to demonstrate the efficiency of the proposed method.

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CP12

Interpreting IDR As a Petrov-Galerkin Method

In this talk, we show that the IDR method of Sonneveld and van Gijzen [*SIAM J. Sci. Comput.*, 31:1035–1062, 2008] can be interpreted as a Petrov-Galerkin (projection) method with a particular choice of left Krylov subspaces; these left subspaces are rational Krylov spaces. Consequently, other methods, such as BiCGStab and ML(s)BiCG, which are mathematically equivalent to some versions of IDR, can also be interpreted as Petrov-Galerkin methods. The connection with rational Krylov spaces inspired a new version of IDR, called Ritz-IDR, where the poles of the rational function are chosen as certain Ritz values. Experiments are presented illustrating the effectiveness of this new version.

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CP13

Charge Retrieval Analysis for Lightning Flashes in a Mountain Thunderstorm

On 24 August 2007, a balloon was launched from Langmuir Laboratory, NM. An electric field sonde (Esonde) measured the electric field during the flight, while simultaneously Lightning Mapping Array recorded the location of VHF pulses generated during lightning. The Esonde and LMA data are the basis for an inverse problem whose solution yields the charge transport due to a lightning stroke. The analysis of several interesting flashes provides new insight into charge transport processes in a thunderstorm.

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CP13

An Adaptive Mesh Refinement Strategy for Finite Volume Methods

In this talk we will present a goal-oriented adaptive mesh refinement strategy for finite volume methods. The strategy is based on the a posteriori error analysis of the numerical solution using the duality between the primal equation and the adjoint equation. This approach has two major advantages: one is that it does not require the numerical method to be in a variational form, for which most FVMs are not; the other is that the well-posedness of the adjoint problem can be studied using standard PDE theories. Examples in 1D and 2D will be shown. When time permitting, the application of such strategy to regional modeling will be discussed.

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CP13

Equilibrium Conditions and Sound Velocities in Two-Phase Flows

We consider a hierarchy of hyperbolic models describing single-component two-phase flows in pipelines, with applications to CO_2 capture and storage. The hierarchy is characterized by the number of equilibrium assumptions made. We present a formal proof that every additional level of enforced equilibrium lowers the propagation velocity of pressure waves. This subcharacteristic condition holds for arbitrary thermodynamic state equations. We present numerical examples relevant for CO_2 transport, and argue the importance for pipeline integrity simulations.

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CP13

Nonlinear Homogenization Problem in the Acoustics of a Two-Phase Medium

Effective equations modeling the acoustics of a two-phase medium with periodic microstucture are derived. The medium (such as cancellous bone) is composed of a linear viscoelastic matrix filled with non-Newtonian fluid. Nonlinear governing equations are obtained via two-scale homogenization and other weak convergence techniques. The effective model is a two-velocity system for the effective velocity v and a corrector velocity w. The effective stress is explicitly dependent on the sum of the strain rates.

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CP14

H_2-Optimal Interpolation: New Properties and Applications

H_2-optimal interpolation points have received great attention recently due to their success in producing accurate reduced-order models in a numerically efficient way. In this talk, first, we will show how H_2 optimal interpolation points can be applied to optimal H_∞ model reduction. Second we consider their potential-theoretic properties and connection to the rational Zolotarev problem. Thirdly, we consider how they behave in the ADI iteration and connect this to projection methods for solving Lyapunov equations.

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CP14

A Characterizaton of ${}^2D_n(q)$ by Order of Normalizer of Sylow Subgroups

Let (V, f) be a orthogonal space, where $V = V_{2n}(q)$, f is a nondegenerate orthogonal form and there are maximum $(n-1)$ distinct hyperplanes in V. Define $SO^-_{2n}(q) = \{A \in SL_{2n}(q) \mid f(Av, Aw) = f(v, w) \text{ for all } v,\ w \in V\}$ and ${}^2D_n(q) = \Omega^-_{2n}(q)/Z$, where $\Omega^-_{2n}(q) = (SO^-_{2n}(q))'$ and Z is the center of $\Omega^-_{2n}(q)$. In this paper, we characterize the simple group ${}^2D_n(q)$ by the order of normalizer of its Sylow subgroups.

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CP14

Measuring the Connectedness of Geographically Embedded Graphs

Many networks surround us share the property that there exists underlying metric space in which the nodes are embedded in. For example, neurons in the brain, or flight connections. To measure the efficiency one can navigate in such networks with only local information, we introduce the concept of greedy connectivity for such geographical networks. By using a chemical potential like parameter, the greedy connectivity accounts also for imperfect transmission across established links.

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CP14

On the Largest Eigenvalue of Distance Matrix of Some Nanotubes

Let G be a connected simple graph with set of vertices $V(G) = \{v_1, \ldots, v_n\}$. The distance matrix $D(G)$ of G is a square matrix of order n, whose entry d_{ij} the between the vertices v_i and v_j in G. The eigenvalues of $D(G)$ are denoted by $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$. Since the distance matrix is symmetric, its eigenvalues are real numbers and can be ordered as $\mu_1(G) \geq \mu_2(G) \geq \ldots \geq \mu_n(G)$.

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CP14

You Can't Beat Gibbs and Runge

Suppose you sample an analytic function f in n equispaced points in $[-1, 1]$. Can you use this data to approximate f in a manner that converges exponentially as $n \to \infty$? Many algorithms have been proposed that are effective for practical values of n, but we prove that they must all fail in the limit $n \to \infty$: exponential convergence implies exponential ill-conditioning.

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CP14

Application of Fractional Calculus to the Analysis of Laplace Transformed Data

This paper describes a novel method using fractional calculus to estimate non-integer moments of a random variable from the measured Laplace transform of its probability density function. We demonstrate that the ω-th moment ($\omega \in \mathbf{R}$) of the random variable can be directly obtained by a linear transformation of the data. When $\omega > 0$, computation of moments corresponds to fractional integration of the data. When $\omega \leq 0$, computation of moments corresponds to fractional differentiation.

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CP15

Optimal Control of a Stochastic Volterra Integral Equation in Hilbert Space with Fractional Brownian Motion Input

This paper investigates stochastic Volterra integral equations in Hilbert spaces. The existence and uniqueness of their adapted solutions is established. The regularity of the adapted solutions to these equations is proved by means of Malliavin calculus. For an application, we study an optimal control problem for a stochastic Volterra integral equation with Hilbert space-valued fractional Brownian motion input. A Pontryagin-type maximum principle is formulated for the problem, and an example is presented.

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CP15

A Computational Measure Theoretic Approach to Inverse Sensitivity Analysis

We consider the inverse sensitivity analysis problem of quantifying the uncertainty of inputs to a finite dimensional map given specified uncertainty in a linear functional of the output of the map. Our formulation is based on the Law of Total Probability that represents a direct inversion of the forward stochastic sensitivity problem for a deterministic model. We derive and analyze an efficient computational measure theoretic approach to approximate a probability measure on the input space.

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CP15

Large Deviation of Quantum Markov Semigroups.

It has been found recently in a series of papers by F. Fagnola and R. Rebolledo that the time averages of a Markov semigroup of completely positive linear maps acting on a von Neumann algebra converges in weak* topology to a stationary quantum state and that necessary and sufficient conditions have been established for the faithfulness of the stationary state. In this paper we obtain a large deviation principle for this convergent sequence. The rate function for large deviation is also established.

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CP15

Analysis of Centralized Sequential Probability Ratio Test (SPRT)-Based Models for Group Decision-Making

Centralized group decision-making models are of interest because important decisions are frequently made by a committee. Our goal is to analyze the relative benefits of different group decision rules, in terms of speed and accuracy. We model the individuals in our group with the SPRT, an optimal and biologically-relevant method, then combine the individual decisions to arrive at the group decision. We will present both analytical and computational results.

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CP15

Evaluating Expectations of Functionals of Brownian Motions: a Multilevel Idea

Pricing a path-dependent financial derivative, such as an Asian option, requires the computation of $E[g(B(\cdot))]$, the expectation of a payoff functional, g, that depends on a Brownian motion, $(B(t))_{t=0}^{T}$. This problem turns out to be an infinite dimensional problem. A multilevel algorithm with low discrepancy designs is introduced to approximate the infinite dimensional integral. The worst case error as a functional of each level's sample size and truncated dimension is minimized. Numerical examples in computational finance will be presented.

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CP15
Benchmark Approach for Defaultable Claims

We study the benchmark approach for defaultable claims. The local risk minimizing strategy is derived in the case when the agent information takes into account the possibility of a default event. Here we do the pricing and hedging of the defaultable claim under the real world probability measure only.

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CP15
Convergence of Tau Leaping Schemes for Markov Jump Systems on a Lattice

Tau leaping methods provide an efficient way to simulate Markov jump systems on a lattice. Existing convergence results on tau leap methods apply only to systems that remain in a bounded region and/or are specific to the explicit and the implicit tau leap schemes with Poisson random variates. We present new convergence results that deal with fairly general tau leap schemes applied to unbounded systems that possess certain moment growth bounds.

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CP16
Convergence of Discontinuous Time-Stepping Schemes for the Gradient Minimization Boundary Control Problem

The minimization of the energy functional having states constrained to semi-linear parabolic PDE's is considered. The controls act on the boundary and are of Robin type. The discrete schemes under consideration are discontinuous in time but conforming in space. Stability estimates are presented at the energy norm and at arbitrary times for the state, and adjoint variables. The estimates are derived under minimal regularity assumptions and allow us to prove onvergence of the discrete solutions.

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CP16
Active Incipient Fault Detection With Multiple Simultaneous Faults

The problem of detecting small parameter variations in linear uncertain systems due to incipient (slowly developing) faults is considered. Using an active fault detection approach, an input signal is injected into the observed system in order to enhance detection of faults. Unlike previous studies where it is usually assumed that there is only one fault occurring at a time, we allow for multiple faults to occur simultaneously which is a natural assumption in the incipient case. A computational method for the construction of an optimal input signal for achieving guaranteed detection with specified precision is presented. This work is an extension of the multi-model approach used for the construction of auxiliary signals for incipient failure detection. There are both discrete time and continuous time versions of this problem. The discrete time case with a modified noise bound is examined. The continuous time case with a similar model that requires solving a linear quadratic regulator problem is also studied. Both models involve only additive uncertainty.

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CP16
PageRank Optimization Through Ergodic Control

We study a general class of pagerank optimization problems, which consist in finding an optimal outlink strategy for a web site subject to design constraints. We model these problems by constrained Markov decision processes, in which the webmaster determines the transition probabilities of websurfers. We identify assumptions under which there exists a "master' page to which all controlled pages should point. We report numerical results exploiting dynamic programming and convex programming techniques.

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CP16
Adaptive and Higher Order Numerical Solution for Optimal Control of Monodomain Equations in Cardiac Electrophysiology

The focus of this work is on the development and implementation of an efficient numerical technique to solve an optimal control problem related to a reaction-diffusions system arising in cardiac electrophysiology. A Newton-type method for the monodomain model, which is a well established model for describing wave propagation of the action potential in the heart, is developed. The numerical treatment is enhanced by using a second order time stepping method, adaptive grid refinement techniques and receding horizon methods. A super linear convergence is achieved for Newton's optimization algorithm.

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CP16

Why Walk and Run: Towards a Predictive Theory of Legged Locomotion Based on Energy Optimality

Healthy human legs are capable of great behavioral complexity – some human legs are capable of even "breakdancing". But mostly, people use stereotypical gaits – "walking" at low speeds and "running" at high speeds. Why these particular gaits from among the millions our legs are capable of? Using optimal control calculations using a simple mathematical model and classic prior experiments, I will show evidence that the patterns of movement that we use roughly minimize energy cost of locomotion. I will show how to extend this simple theory to obtain better quantitative predictions of people walk and run.

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CP16

Efficient Loudspeaker Horn Design: from Mathematical Model to Experimental Validation

During the last few years, we have designed numerous acoustic devices using gradient-based boundary shape and topology optimization. This talk outlines strategies to optimize acoustic devises with respect to efficiency and directivity properties. The acoustical properties are calculated through numerical solutions of the Helmholtz equation. Recently, we manufactured one of our designs and analyzed it in an anechoic chamber. In the design frequency band, the acoustic impedance is close to ideal.

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CP17

Modeling Complex Fluid Flows in Porous Media

Flow of complex fluids in porous media occurs in many processes, some naturally occurring and some by design. Modeling of such flows accurately and efficiently is a non-trivial task. We will discuss in this talk many non-trivial issues that come up in the context of setting the correct mathematical model that includes myriad effects that play a role. In this context we may take some simple model problems and show some exact and computational results. This is an ongoing work.

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CP17

Multiscale Modeling of Heterogenous Flow with Non-Newtonian Behavior

A new multiscale approach to modeling non-Newtonian /heterogenous flow will be discussed. The computations are carried out by combining an Immersed-Boundary-Method with Brownian Dynamics. The exchange of information between both computational techniques is done through the velocity gradient and stress state tensors. Several examples will be presented including the response of a Newtonian drop suspended in a viscoelastic fluid and the dynamics of Newtonian bubbles rising in a viscoelastic fluid.

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CP17

Three-Dimensional Multispecies Nonlinear Tumor Growth: Tumor Invasion and Angiogenesis

We study 3D non-linear tumor growth by tracking multiple viable cell species populations, discrete angiogenesis vessels and individual cell movement using a hybrid continuum-discrete approach. We investigate disease progression as a function of cellular-scale parameters such as proliferation and nutrient uptake rates in both avascular and vascular regimes. We find that heterogeneity in the physiologically complex tumor microenvironment can be quantitatively linked to the tumor macro-scale as a mechanism that promotes morphological instability.

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CP17

Eulerian Formulation of Fluid/structure Interaction

The interaction of an elastic structure and a fluid occurs in many phenomena in physics. To avoid the difficulty of coupling lagrangian elasticity and eulerian fluid we consider a whole eulerian formulation. The elasticity of the structure is computed with retrograde caracteristics which satisfy a transport equation and a level set function is introduced to capture the interface between the fluid and the structure. In application, we will present some numerical simulation relative to biolocomotion.

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CP17

A Parallel Monolithic Approach for Blood Flow Modeling

We study a parallel algorithm for the simulation of blood flows in arteries using a coupled system of PDEs consisting of incompressible Navier-Stokes equations and a linear elastic equation. The coupled nonlinear system is solved by a Newton-Krylov algorithm preconditioned by an overlapping Schwarz method. We focus on the investigation of the algorithm for different outflow boundary conditions, and also on the scalability of the software on computers with a large number of processors.

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CP17

A Hybrid Numerical Method for Two-Phase Flow with Soluble Surfactant

We present a hybrid numerical method for computation of fluid interfaces with soluble surfactant at large bulk Peclet number. A narrow transition layer adjacent to the interface which is important in controlling the interface dynamics is resolved by introducing a singular perturbation reduction of the transition layer into full numerical solution of the free boundary problem. Numerical results are presented for two-phase flows in the Stokes flow limit.

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CP18

On Accurate Reduced-Order Modeling Using Proper Orthogonal Decomposition

Reduced-order models based on the proper orthogonal decomposition (POD) are often used to represent a complex dynamical system in fluid flows. However, for Navier-Stokes equations, these models have been successfully developed mainly for 2-D flows and are limited to a reference simulation. We present improvements in the reduced-order model to expand its applicability and encounter various stability issues in the model. We then compare results of reduced-order models with direct numerical simulations.

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CP18

Semiclassical Asymptotics in Norm for Non-Smooth and for Nonlinear Problems

Quantum problems, formulated appropriately, are well known to converge to their classical counterparts as Planck's constant $\hbar$ tends to zero. On a mathematical level, this is traditionally seen as a weak-$*$ proximity between the solutions of the quantum and classical phase-space kinetic equations (Wigner and Liouville respectively). Indeed a lot is known for the weak-$*$ convergence to the semiclassical limit, both for linear and nonlinear problems with sufficient smoothness. However, much less is known for strong topology approximations; the first systematic exploration of H^s convergence, for linear problems, appeared in 2006. In this work we show semiclassical approximation results, for the linear case (for pure and mixed states), in the H^s, $s \in \mathbf{Z}$, norms, with weaker assumptions than the state of the art. Moreover, in certain cases we can lower the smoothness assumptions enough for our results to be applicable to $C^1 \setminus C^{1,1}$ potentials. In such problems the weak-$*$ approximation is known to hold, but the limit Liouville

equation has multiple solutions: the semiclassical limit is known to be *a (weak)* solution of the Liouville equation, but *which one* is not known. In a family of such problems, we can choose the solution of the Liouville equation which corresponds to the limit of the Wigner equation. Moreover, for the first time to the best of our knowledge, we show an L^2 semiclassical limit for mixed states evolving under the Hartree equation, i.e. we show that the solutions of the Wigner-Poisson equation and the nonlinear Vlasov equation are close in L^2 as $\hbar$ tends to zero. These results are joint with T. Paul, M. Pulvirenti and F. Pezzoti, and use heavily the technique of the smoothed Wigner transform.

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CP18

On the Right Hand Side Identification Problem for a Parabolic Equation with Nonlocal Conditions

We consider the inverse problem of reconstructing the right side of a parabolic equation $\frac{\partial u(t,x)}{\partial t} = \frac{\partial}{\partial x}\left(k(x)\frac{\partial u(t,x)}{\partial x}\right) - \sigma u(t,x) + \eta(t)\psi(x),\ 0 < x < l,\ 0 < t \leq T,$ $u(t,0) = u(t,l), u_x(t,0) = u_x(t,l), 0 \leq t \leq T,\ u(0,x) = u_0(x),\ 0 \leq x \leq l, u(t,x^*) = \varphi(t),\ 0 \leq x^* \leq l, 0 \leq t \leq T$, where $u(t,x)$ and $\eta(t)$ are unknown functions and $k(x) \geq \delta > 0$ and $\sigma > 0$. Under the applicability conditions, well-posedness of this problem is investigated. A numerical algorithm for the approximate solution of the problem is presented.

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CP18

An Extended State Approach to Online Parameter Identification in Parabolic Pdes

Existing techniques for estimating model parameters in time-dependent partial differential equations simultaneously to the time evolution of the physical state exclude the case of partial state observations or require to solve online Ricatti type operator evolution equations. We suggest and analyze an extended state approach to online parameter identification in a class of possibly nonlinear parabolic PDEs that avoids Ricatti type equations but still allows for partial state observations. Numerical examples underline the feasibility of our method.

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CP18

Maximum Principles and Bounds for Some Semilinear Fourth Order Partial Differential Equations

We consider several classes of elliptic, semilinear fourth order partial differential equations from plate theory. We use classical maximum principles to deduce that certain functionals defined for the solution of these equations achieve their maximum value on the boundary of the domain. Bounds on various quantities of interest are then deduced.

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CP18

The Effect of Upscaling on Seismic Inversion

Small-scale geologic features may have a large impact on estimates of material parameters determined by seismic inversion. Unfortunately there is no magic scale known a priori on which the important features of the subsurface reside. Two-scale forward modeling leads to interesting questions about model parameter estimation. In the case of constant density acoustics, studies indicate the estimated sound velocity should correspond to an average, but numerical experimentation is required in the case of variable-density acoustics.

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CP19

Stability Results on Multi-Layer Hele-Shaw Flows

We will present stability results on multi-layer Hele-Shaw flows in cases where layers may have either uniform or non-uniform properties. These results can be harnessed for stabilization purposes. Theoretical and numerical studies reveal some interesting properties about instability transfer mechanism between different interfaces.

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CP19

Century-Timescale Rossby Waves in the Arctic Ocean

A number of co-existing oceanographic and atmospheric systems interact with quite different timescales in the evolution of the global climate. It has been suggested that the approximately circular arctic ocean might support a century-timescale, ocean-layer Rossby (planetary) wave, which could interact with the north Atlantic circulation. We investigate the modeling, dynamics and spectral properties of such a wave. Joint with T. Schmidt (Danish Meterological Institute), and M. Petersen, (DTU Mathematics).

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CP19

Storm Surge Simulations Using Adaptive Mesh Refinement

We present preliminary results of storm surge simulations with idealized bathymetry and hurricane model data with adaptive mesh refinement. The goal of this study is to gain an understanding of how adaptive mesh refinement could provide greater computational efficiency and higher resolution than traditional methods used to model these phenomena. Multi-layer methods are also investigated in order to include basic three dimensional affects in the simulation.

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CP19

Accuracy of Tail Regions in Uncertain Climate Model Predictions

Conventional spectral methods for uncertainty quantification are generally challenged in the "tails" of input distributions. Extensive sampling in the tail regions is especially costly in climate models. We will illustrate how the usage of non-conventional basis functions and surrogate model analysis improves the convergence of the spectral expansions in the tail regions. Preliminary results will be shown for the Atlantic meridional overturning circulation shutoff case as a result of abnormally high climate sensitivity values.

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CP20

Multifrontal Multithreaded Rank-Revealing Sparse QR Factorization

SuiteSparseQR is a sparse QR factorization package based on the multifrontal method. LAPACK and the multithreaded BLAS are used within each frontal matrix. Parallelism across different frontal matrices is handled with Intel's Threading Building Blocks library. Rank-detection is performed within each frontal matrix using Heath's method. The resulting sparse QR factorization obtains a substantial fraction of the theoretical peak performance of a multicore computer. The method is used in backslash in MATLAB for sparse rectangular matrices.

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CP20

Fast Computation of Schur Complements of Large Finite Difference Matrices

It is well-known that the linear equations associated with finite difference operators on structured grids admit very fast solution techniques. Recently developed fast direct solvers require much less memory than FFT for constant coefficient operators, and are more robust than iterative techniques in the general case. The direct solvers are also extremely fast for problems with multiple right-hand sides. We will present fast methods for computing Schur complements of a finite difference matrix.

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CP20

Parallel Solution of Large Symmetric Eigenvalue Problems Via Trace Minimization

The Trace Minimization algorithm (TraceMIN) is a symmetric eigenvalue problem solver that minimizes the trace over a subspace. TraceMIN requires the solution of a set of linear systems with modest accuracy. In this talk we present the convergence properties and the parallel scalability of a new version of TraceMIN. In addition, we compare the parallel performance of our algorithm with PARPACK for solving eigenvalue problems that arise in MEMS device simulation and other applications.

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CP20

New Results in Numerically Solving Large-Scale Algebraic Sylvester Equations

Two approaches are investigated for constructing numerical solutions of large-scale Sylvester equations. The first is to transform the Sylvester equation into an invariant subspace problem, which can be solved efficiently in real arithmetic. Optimal shift selection is presented to enhance convergence of iterative eigensolvers. This optimal shift selection analysis is then generalized for the computation of

multiple optimal real shifts for the ADI approach, resulting in a more compact search region for the optimal shifts.

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CP20

Piro_sky: Pipelined Rotations for Sparse Skyline Svd

PIRO_SKY is a library for computing all the singular values of a sparse matrix efficiently. PIRO_SKY uses sparse data structures and blocked algorithms to compute the singular values. The impact of various profile reduction ordering strategies on computing the sparse SVD will be discussed. We show PIRO_SKY is competitive against iterative methods even when only a reasonable number of singular values are required. We also present the software engineering aspects of PIRO_SKY's design.

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CP21

Numerical Tests of An Algorithm for Seismic Imaging and Inversion

We present numerical tests for an acoustic inverse scattering algorithm for simultaneous geophysical imaging and amplitude correction from measured data. No knowledge about the medium under investigation is assumed. We model the data from several one-dimensional earth configurations and show how the algorithm can find the precise location and a good estimate of the layers' parameters from data only. Our tests will include different number of layers, high/low contrasts, velocity inversions and noisy data.

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CP21

Reduced Order Modeling to Enhance Thermal Imaging for Crack Detection

Proper orthogonal decomposition is employed as part of an algorithmic means to identify micro-cracks in metal plates. As model-updating approaches are used to solve the resulting inverse problem, POD offers relief from the ensuing computational challenges. A new approach to incorporating POD modes, as an enrichment to the finite element basis functions used in the forward models, will be treated.

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CP21

System Identification in Tumor Growth Modeling

Several theoretical efforts were devoted to setting up phenomenological models describing cancer propagation. Among them models based on partial differential equations describe macroscopic and mechanical features of tumor propagation on the basis of mixture theory. Such models are parametric but parameters cannot be fixed *a priori* because they do not derive from first principles. Also, they cannot be measured directly because they represent mesoscale properties. In order to approach realistic applications, *i.e.*, provide a prognosis or a therapy evaluation tool, realistic values for these parameters must be found. The aim of this work is to present an efficient procedure to solve data assimilation problems, the data coming from medical imagery. Several realistic cases are analyzed, showing that the prognosis can be accurate on a significant time scale.

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CP21

A Lagrangian Scheme to Solve the Monge-Kantorovich Problem

The Monge-Kantorovich problem was recently rediscovered and studied, having applications in statistics, meteorology, numerical optimization, physics, medical imagery. In the literature three family of solution methods were proposed: the first class is based on the Kantorovich duality, the second one on the continuous formulation and the third one on the critical points of a dynamical flow (AHT). In this work we propose a different approach: we implicitly satisfy the transport equation by propagating mass particles on rays. Particle discretization makes the integration simpler and the parallelization efficient. Several 2D and 3D cases are presented.

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CP21

Simultaneous Imaging and Inversion Using An Inverse Scattering Algorithm

We present a method, derived from inverse scattering theory, for geophysical imaging and amplitude correction from measured data. No knowledge about the medium under investigation is assumed. Although derived as a series, the algorithm is shown to converge to a closed form independent of the parameters involved in the problem. Analytic and numerical one dimensional examples show excellent results in finding both the location of interfaces and the amplitude of acoustic reflections.

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CP21
Semi-Blind Deconvolution in 4Pi-Microscopy

4Pi-microscopy has been invented by Stefan Hell to improve the resolution of confocal fluorescence microscopy along the optical axis. The convolution kernel (or point spread function, short psf) of a 4Pi-microscope differs from the psf of a corresponding confocal microscope approximately by a squared cosine factor resulting in a main peak of much smaller band-width and several (typically at least two) side lobes. The size and position of the main peak and the side lobes of the 4Pi-psf depend on a phase parameter, which has been assumed to be space-invariant so far, yielding standard deconvolution problems with positivity constraint. However, this assumption is violated e.g. for inhomogeneous refractive indices, and the space dependence of the psf is considered as one of the main problems in 4Pi-microscopy. In this project the joint recovery of the three-dimensional density of fluorescent markers and the slowly varying phase function is considered as a nonlinear inverse problem, which is tackled by a variant of the iteratively regularized Gauss-Newton method (IRGNM) respecting the positivity constraint. We present a convergence proof for this constraint IRGNM and reconstruction results for artificial and real data.

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CP21
Attenuation Compensation and Boundary Segmentation in Ultrasound Images

Spatial variations of attenuation across tissue can result in shadowing and enhancement in ultrasound B-scan images. These artifacts affect the underlying signal backscatter which is the main component of ultrasound images and has clinical significance in detecting diseases and tumors. We present a joint estimation method based on the variational principle to compensate for attenuation artifacts via functional minimization and regularization. Pair of pathological useful backscatter and attenuation fields is reconstructed along with segmented anatomic structures.

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CP22
The Numerical Stability of Reorthogonalized Block Classical Gram-Schmidt

A reorthogonalized block classical Gram–Schmidt algorithm is given that factorizes a full column rank matrix A into $A = QR$ where Q is left orthogonal (has orthonormal columns) and R is upper triangular and nonsingular. With appropriate assumptions on the diagonal blocks of R, the algorithm, when implemented in floating point arithmetic with machine unit ε_M, produces Q and R such that $\|I - Q^T Q\|_F = O(\varepsilon_M)$ and $\|A - QR\|_F = O(\varepsilon_M \|A\|_F)$. The resulting bounds also improve a previous bound by Giraud et al. [Numer. Math. 101:87–100,2005] on their CGS2 algorithm.

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CP22
Polynomial Transform Decomposition Using Module Induction

Polynomial transforms, or generalized Vandermonde matrices, are an important class of matrix-vector products used in mathematics and engineering. Important examples include the discrete Fourier transform, discrete cosine and sine transforms, and transforms related to orthogonal polynomials. We present a novel method to derive fast transform algorithms by decomposing the associated polynomial algebra using a technique from representation theory called induction. The method algebraically characterizes and generalizes transform algorithms reported in the literature.

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CP22
A Schur Complement Approach for Solving a Nearly Hermitian System

We discuss an approach for solving an $n \times n$ linear system with rank s skew-Hermitian part ($s \ll n$). This can be interpreted as the Schur complement of a larger $(n + s) \times (n+s)$ system. We can solve the original system by solving $s+1$ Hermitian systems, e.g., using MINRES, and directly solving one $s \times s$ system. We present a bound for the outer residual norm in terms of residuals of the Hermitian systems and develop a suitable stopping criteria.

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CP22
Numerical Stability of a Complete CS Decomposition Algorithm

A proof of backward stability for the simultaneous bidiagonalization of all four blocks of a partitioned unitary matrix will be outlined. The reduction serves as the first phase in an algorithm for the complete CS decomposition.

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CP22

Fast Inexact Implicitly Restarted Arnoldi Method for Generalized Eigenvalue Problems with Spectral Transformation

We study an inexact implicitly restarted Arnoldi (IRA) method for computing a few eigenpairs of generalized non-Hermitian eigenvalue problems with spectral transformation, where in each Arnoldi step (outer iteration) the matrix-vector product involving the transformed operator is performed by iterative solution (inner iteration) of the corresponding linear system of equations. We provide new perspectives and analysis of two major strategies that help reduce the inner iteration cost: a special type of preconditioner with "tuning', and gradually relaxed tolerances for the solution of the linear systems. The effectiveness of these strategies is demonstrated by numerical experiments.

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CP23

Uzawa Algorithms for Non-Symmetric Saddle Point Problems

This is joint work with Brendan McCracken (REU -2009), and Lu Shu (GEMS-UDEL 2009). We introduce and analyze new Uzawa algorithms for non-symmetric saddle point systems. Typical problems where such systems appear are, for example, in finite element or finite difference discretization of steady state Navier-Stokes systems. Convergence for the algorithms are established based on new spectral results about Schur complements. A new Uzawa type algorithm with variable relaxation parameters is introduced and analyzed in a general framework. Numerical results supporting the efficiency of the algorithms are presented for finite element discretization of the the steady state Navier-Stokes equations. Thanks to NSF.

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CP23

Self-Similar Solutions and Their Instability for Liquid-to-Glass Phase Transitions in Vitrification

Some theoretical aspects of vitrification phase transitions are addressed by modeling the process as an isothermal moving-boundary problem in which the two phases have differing diffusivities. A similarity solution is obtained, its linear stability is examined, and an analytic dispersion relation is investigated, yielding the stability boundaries. Extensions of this work in which the vitrified phase demonstrates subdiffusive behavior also will be discussed and the dynamics and instabilities of this adjusted problem examined.

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CP23

A Singularly Perturbed Formulation of the Quantum-Corrected Energy Transport Model

A scaling reformulation of the quantum-corrected energy transport model is presented. We find that the scaled Debye length as the standard singular perturbation parameter for the classical models is no longer valid for the nano-scale semiconductor devices and that the scaled Planck constant is moderately small. We introduce here a new parameter called the scaled thermal conductivity and modify the standard scaled intrinsic density to include a dependence on potentials. It is numerically shown that the modified intrinsic density and the scaled thermal conductivity are strongly singular for the continuity and energy transport equations, respectively.

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CP23

A Gradient-Augmented Level Set Approach with Subgrid Resolution

Level set methods are versatile interface tracking approaches. Common difficulties are the loss of small structures, an accurate approximation of curvature, and the combination with adaptive mesh refinement. We present a gradient-augmented approach, which advects interfaces with third order accuracy, and admits a second order accurate approximation of curvature, both with optimally local stencils. In addition, the presence of gradient information yields a certain level of subgrid resolution, which is beneficial in the tracking of thin films or droplets. We demonstrate this advantage in fluid dynamics simulations.

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CP23

The Immersed Interface Method for Two-Fluid

Problems

Many problems of fluid mechanics involve the interaction of two immiscible fluids. It is generally difficult or inefficient to simulate each fluid separately using an interface-fitted grid method. In the immersed interface method, a two-fluid problem is formulated as one set of governing equations and simulated on a fixed Cartesian grid. The effect of the two-fluid interface enters the formulation as a singular force and a numerical scheme as jump conditions. In this talk, we will present the principal jump conditions, discuss the difficulties in implementing them, and provide a few options to overcome the difficulties. We will use the two-fluid circular Couette flow to demonstrate the accuracy and efficiency of these options.

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CP24

Transport Effects on Surface Reaction Arrays: Applications to Biosensors

The ubiquity of surface-volume reactions makes knowledge of their kinetics critical. Several biosensors designed to measure rate constants, such as the Flexchip and the dot-Lab, have multiple reacting zones in a single flow channel. A basic unidirectional flow model is developed and solved for typical experimental parameters using perturbation methods. The effect of zone placement along the channel can be quantified in terms of an effective Damköhler number based upon position. Moreover, it is established that zone placement across the channel does not affect the measurements.

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CP24

Learning-Rate-Dependent Clustering and Self-Development in a Network of Coupled Oscillators

We investigate the role of the learning rate in a Kuramoto model of coupled phase oscillators in which the coupling coefficients dynamically vary according to the Hebbian learning rule; here synapses between neurons are strengthened when they fire in synchrony. We show that either one or two synchronized clusters form, depending on the learning rate relative to a critical value. We also comment on the possibility of self-development of neural networks within this model.

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CP24

On the Cellular Volume Regulation in 2-D

The electrical and osmotic effects with ion exchange transport mechanism for the volume regulation are investigated. The osmotic effect is modeled by the relative sliding between fluid and membrane normal to the membrane, which is mediated by the interaction between solute and membrane through immersed chemical potentials. The influence of internal versus external ion concentration in determining the volume of an elastic semi-permeable vesicle is studied with and without electrical effects and/or exchange pumping.

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CP24

Mathematical Model of Self-sustained Firing in Motoneurons After Spinal Cord Injury

The self-sustained firing in motoneurons caused by plateau potentials provide a mechanism to translate short lasting synaptic inputs into long lasting motor output. During the acute stage of spinal cord injury the endogenous ability to generate plateaus is lost; however, during the chronic stage the plateau potentials reappear. Using two-compartment conductance based differential equation model we investigate mechanisms that might contribute to spasticity due to the self-sustained firing.

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CP24

Mathematical Modeling of Cell Biopreservation by Desiccation

We consider the model of a cell with an incompressible water-sugar mixture inside and outside the cell. The cell membrane has resistance to bending and local incompressibility. As water leaves through the surface, a glassy state can be formed inside the cell, whose volume decreases while local area of the membrane is fixed. The hydrodynamics is governed by the Stokes equation. We investigate linear stability and dynamics of an initial spherical membrane.

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CP24

Frequency Modulation of the Excitable Fitzhugh-

Nagumo System

Using a generalized Fitzhugh-Nagumo model we studied how temporal characteristics of an external signal affect the dynamics of excitable systems. In particular, we choose a subset of parameters for the Fitzhugh-Nagumo system so that the solution contains (1) no limit cycle or (2) a unique limit cycle. For this set of parameters, we investigate the dynamic consequences of injecting the system a variable current I(t,w) with different frequency w.

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CP25

Finite Difference Method for Smoothed Gradually Varied Surfaces

A digital method for obtaining continuous functions with smoothness to a certain order ($C^{(n)}$) from sample data is designed. This method is based on gradually varied functions discovered by Chen in 1989 and finite difference method. This new method has been applied to real groundwater data and the results have validated the method. This method is independent from existing popular methods such as the cubic spline method and the finite element method. The new digital-discrete method has considerable advantages for a large amount of real data applications. This digital method differs from the classical discrete method that usually uses triangulations.

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CP25

Lime: Lightweight Integrated Multiphysics Environemnt

LIME is a multiphysics coupling environment that enables coupling of both legacy application codes as well as novel codes. It is lightweight by requiring application codes to only provide a response given requisite inputs. It provides value-added coupling by incorporating any additional information to effect more robust coupling algorithms based on variations of Jacobian-Free Newton-Krylov. LIME is currently implemented as extensions to the Trilinos Solver Framework thereby leveraging state-of-the-art solution algorithms to drive multiphysics coupling.

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CP25

Numerical Computations of Particle-Laden Turbulent Flows

An efficient Eulerian-Lagrangian particle dispersion algorithm for the prediction of particle-laden flows is proposed. The volume fraction of the dispersed phase is assumed to be small enough such that particle-particle collisions are negligible and properties of the carrier flow are not modified. With the examination of dilute systems only the effect of turbulence on particle motion has to be taken into account (one-way coupling). With this assumption the continuous phase can be treated separate from the particulate phase. The continuous phase is determined by large-eddy simulation in the Eulerian frame of reference whereas the dispersed phase is simulated in a Lagrangian frame of reference.

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CP25

Cluster Computing with Intel Nehalem and InfiniBand Interconnect

High performance parallel computing depends on the interaction of a number of factors including the processors, the architecture of the compute nodes, their interconnect network, and the numerical code. In this talk,we present performance and scalability studies on a new 86-node distributed-memory cluster with two quad-core Intel Nehalem processors per node and a quad-data rate InfiniBand interconnect. These components are currently the most popular for general-purpose clusters and they exhibit excellent performance.

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CP25

Nonlinear Evolution of Electrified Liquid Threads and Annular Layers

The nonlinear dynamics of an electrified liquid thread in a cylindrical tube (electrode) which is concentrically placed is studied. The radial electric field is generated by the potential difference between the fluid interface and the outer electrode. We solve the system in the zero Reynolds number limit by the boundary-integral method. Pinch-off solutions and satellite formation are discussed. In addition, different breakup behaviors are found at other parameter values.

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CP25

Mathematical and Numerical Analysis of Peridynamic Models with Nonlocal Boundary Conditions

We study the linear bond-based peridynamic models with a particular focus on problems associated with nonstandard nonlocal displacement loading conditions. Both stationary and time dependent problems are considered for a one dimensional scalar equation defined on a finite bar and for a two dimensional system defined on a square. The related peridynamic operators and associated functional spaces are analyzed. Applications to the analysis of the finite dimensional approximations to peridynamic models are also illustrated.

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CP26

A Differential Equation/agent-Based Hybrid Model of Antibiotic-Resistant Infection in a Hospital Ward

When modeling the spread of bacterial infections in a population, dynamics occur on two levels: Interaction between the people in the ward, and the bacterial growth taking place inside infected ward members. We propose a method for combining both into a single model, where each person is treated as an agent in an agent-based system, with the agent-specific dynamic parameters driven by a differential equations system that models the within-host bacterial dynamics for that agent.

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CP26

Optimal Efficacy of Ribavirin in the Treatment of Hepatitis C

A mathematical model to represent hepatitis C is presented. An objective functional keeping biomedical goals in mind is formulated. The optimal control problem is solved numerically to obtain an optimal efficacy of ribavirin in a combination treatment of ribavirin with interferon, where the efficacy of the latter has a clinically validated functional form

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CP26

Drug Resistance Effects on Weighted Optimal Control for Chemotherapy

A differential equations model for cancer and its treatment is examined. The governing equations are developed from a four-compartmental model that shows the development of resistance over time. Optimal control techniques are then used to investigate the effects of drug resistance (both natural and induced) on cell-cycle specific chemotherapy regimes. Optimal strategies are suggested that take into account factors such as toxicity level. Once the existence of the optimal control is established, the control is then characterized through the Hamiltonian and the adjoint system to governing equations.

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CP26

A Spatiotemporal Model of Barley Yellow Dwarf Virus in Competing Plant Species with Seasonality and Age Structure

Barley yellow dwarf virus infects over 100 grass species in agricultural and natural systems, mitigating success of invasive species. We model BYDV transmission within a metapopulation framework incorporating the movement of aphid vectors between discrete host patches. We examine BYDV persistence and alteration of pathogen-mediated interactions between perennial and annual competitors across a range of host community configurations. Sensitivity analysis of the basic reproduction number for two simplified models identifies how key parameters influence pathogen invasion.

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CP26

Control of Mosquito Populations Through the Introduction of Sterile Mosquitoes

We construct an ODE model for the release of sterile mosquitoes into a population of wild mosquitoes. Assuming Holling-II dynamics, we examine the optimal control of the wild mosquito population through several objective function formulations. Numerical simulations are discussed.

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CP26

Phase Locking Between the Expression Profiles of Transcription Factors and Their Target Genes During the Yeast Cell Cycle

Increasing evidence now suggest the role of frequency modulation in gene expression. We examined this question using the time course gene expression data of yeast cell cycle. We found that between transcription factors and their binding targets, the expressions are significantly more likely to be phase locked than random gene pairs. In addition, ~ 5–10% show higher order, more than $1:1$, phase locking.

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CP27

Quantitative Dynamics of Spiral Waves in Active Media.

If perturbed, spiral waves in active media slowly move their core. In linear approximation, the drift velocity is proportional to convolution of perturbation with translational response function (RF), the eigenfunction of adjoint linearized operator corresponding to translational symmetry. For variety of perturbations, we compute drift velocities using RFs in Barkley and FitzHugh-Nagumo models and show good quantitative agreement with direct numerical simulations. We also demonstrate orbital movement of spiral due to interaction with localized inhomogeneities.

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CP27

Complex Media, Complex Fluids and Complex Flows

Flows involving simple fluids are relatively well understood in comparison to complex fluids such as blood, petroleum, jam, honey, just to cite a few. In fact, many of the biologic, edible, and chemical fluids are complex in nature. Many such fluids are product of nature and many are man made by design in order to achieve some specific objectives. For example, complex fluid such as aqueous solution containing polymer and surfactants are used in improved oil recovery processes.It is necessary to understand at the fundamental level the origin of many physical phenomena that can be triggered by the complex rheological properties of these complex fluids, in particular in complex media. Such understanding can lead to better design of many processes and better numerical methods to simulate these processes.

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CP27

Turing Patterns with External Morphogen Gradients

In embryonic development, cells self-organize into complex distributions giving rise to tissues and organs. The basic mechanisms of how this happens are still not very well understood. One experimentally verified mechanism is the action of gradients of signalling molecules. Another one is the Turing mechanism in reaction-diffusion systems. To investigate how these two mechanisms may interact, we propose a generic model of a reaction-diffusion system in the presence of a morphogen gradient. This morphogen gradient is established independently of the reaction-diffusion system and acts by increasing the production of the activator proportional to the morphogen concentration. The model is motivated by several existing models in developmental biology in which a Turing patterning mechanism is proposed and various chemical gradients are known to exist. We investigate how the Turing pattern is affected, if it exists. We also apply our results to a model of bone pattern formation in vertebrate limbs and show how they may shed light on some experimental findings.

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CP27

Spatial Modeling of Bacterial Antibiotic Tolerance

Persisters are phenotypic bacterial variants which exhibit "antibiotic tolerance": persisters survive when exposed to bactericidal antibiotics, but the bacterial colonies regrown from persister cells remain susceptible to killing by further antibiotic treatments.Persister formation has been linked to quorum sensing, the ability of bacteria to determine their local population density, and with the formation of biofilms, surface-growing bacterial communities particularly difficult to eradicate with antibiotic treatments. Extending a previous model of bacterial colony pattern formation, we present a reaction-diffusion model of bacterial growth which includes density-dependent persister formation. The model also exhibits separation of temporal and spatial scales between persister and regular bacteria. We investigate the pattern formation properties of the model as a number of experimentally accesible parameters are varied.

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CP27

Mathematical Analysis of a System of Pde Arising From Epidermal Wound Healing

Systems of reaction-diffusion equations have been proposed to study cell migration across the surface of an epidermal wound. Approximation of traveling waves which describe the cell migration into the wound has been studied by a number of researchers. We will investigate asymptotic behavior and speed of the travel wave solutions. Analysis of the model system reveals biological interactions in the wound healing process and the role of the model parameters in determining the speed.

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CP27

Analysis of Equations with Nonlinear Dispersion

At this time, there is little existence theory for equations in which the mechanism which generates dispersion is itself nonlinear. In this talk, I will present a new equation which possesses compactly supported traveling wave solutions (a hallmark of degenerate dispersive equations) and for which the Cauchy problem has a weak solution. This work is joint with D. Ambrose.

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CP28

Mathematical Analysis of Swarming: Integrating Agent-Based Simulation with Population-Level Modeling and Analysis

An agent-based model is used to inform the design of a biologically relevant continuum model for swarming. Linear stability analysis reveals the existence of low-frequency instabilities as key behavioral parameters are varied. The results of the stability analysis are verified via numerical simulation of the continuum model. Simulations of the agent-based model demonstrate a correspondence for finite swarms and are used to evaluate the effects of noise and changes in communication on stability.

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CP28

Mathematical Modeling and Analysis of a Continuum Model for Three-Zone Swarming Behavior

Swarms in nature have been modeled with individuals but a continuum model, in which individuals are replaced with fields, may be better suited to theoretical analysis and scaling up to larger swarms. Models including zones of repulsion, orientation, and attraction are popular in ecological modeling. Our integro-differential equations describe the reactions to the varying density in these three zones. We use linear stability analysis to explore first and second order models of constant density swarms.

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CP28

Nonlinear Dynamics of Coupled Droplet Oscillators

A network of n coupled spherical-cap droplet oscillators is considered. The coupling by inviscid flow between droplets is modeled as a system of $n-1$ second-order differential equations under a constant-volume constraint. For S_n symmetric coupling, analytic stability and bifurcation results are obtained for an arbitrary number of droplets. Nonlinear dynamics are explored numerically in both undamped and weakly-damped cases. In addition, the influence of a variety of coupling laws is analyzed.

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CP28

Robustness and Efficiency of Ant-Based Routing and Forwarding Protocols.

Ant-based protocols provide elegant solutions to routing and forwarding problems. These protocols use control packets or "ants" to discover new routes and reinforce efficient routes by adjusting pheromone values. We revisit the new nonlinear stochastic models and compare them to network simulations with high-fidelity protocol, and physical layer models. Through analysis of the models, we can understand how network behavior depends upon routing exponents and pheromone deposition/evaporation parameters.

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CP28

Dynamics of Light Beam Switching at the Interface of Two Nonlinear Optical Media

The dynamics of two light beams interacting at an interface separating tow nonlinear optical media is studied numerically and analytically. The beam dynamics is simulated by the beam propagation method. The numerical simulations agree with the results of analytical model. The trapped beam at the interface acts as a power controllable switch to reflect or transmit the incident beam at the interface. Some new results will be presented in this talk.

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CP28

High-Order Bisection Method for Computing Invariant Manifolds of 2-D Maps

We describe an efficient and accurate numerical method for computing smooth approximations to invariant manifolds of planar maps, based on geometric modeling ideas from Computer Aided Geometric Design (CAGD). The unstable manifold of a hyperbolic fixed point is modeled by Bézier interpolant (a Catmull-Rom spline) and properties of such curves are used to define a rule for adaptively adding points to ensure that the approximation resolves the manifold to within a specified tolerance. Numerical tests on a variety of example mappings demonstrate that the new method produces a manifold of a given accuracy with far fewer calls to the map, compared with previous methods. A brief introduction to the relevant ideas from CAGD is provided. Additionally, we will discuss the difficulties of extending these ideas to higher dimensions.

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MS1

Absorbing Boundary Condition Taking into Account the Grazing Modes

We propose a new Absorbing Boundary Condition for the wave equation, which is adapted to arbitrarily-shaped convex boundary. After having decomposed the exact solution into propagating, evanescent and grazing fields, this condition is obtained by combining the approximations of the transparent condition in the three corresponding regions. The absorption of the grazing field involves a fractional derivative in space which requires a specific discretization in order to implement the condition in a finite element scheme.

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MS1

A

High Order Runge-Kutta Discontinuous Galerkin Scheme with Time Accurate Local Time Stepping

A new explicit RK based method for the time integration of the DG scheme is presented. The considered class of RK schemes have the property that a time polynomial of the solution is available, which can be used to introduce local time stepping. Despite the local time steps, the scheme is high order accurate in time, conservative and ideally suited for massively parallel computations, allowing an efficient discretization of large scale time dependent problems.

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MS1

Machine-adapted Methods: High-order Wave Propagation on GPUs

Having recently shown that high-order unstructured discontinuous Galerkin methods are a spatial discretization that is well-matched to execution on GPUs, in this talk we explore both novel and traditional supporting components of high-order linear and nonlinear wave solvers for their suitability for modern massively parallel computer architectures. Components examined range from time steppers to preconditioners, linear solvers and shock capturing schemes, for which we examine design considerations, algorithms, and performance data.

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MS1

An Accelerated Discontinuous Galerkin Method for Time-Domain Wave Propagation on Curvilinear Domains

We will introduce the low storage curvilinear discontinuous Galerkin (DG) method for solving time-dependent partial differential equations on curvilinear domains. We will present a proof of stability and show results that indicate the method is typically as accurate as standard DG discretizations on curvilinear domains. Finally we will discuss how this approach has enabled three dimensional electromagnetic scattering and also fluid flows to be computed on a workstation using commodity graphics processing units.

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MS2

Model Reduction of Large Scale System in Oil Industries

Large-scale numerical models for suburface hydrocarbon flow are frequently used during the design phase of oil fields. Moreover, an emerging technique is the use of such models during the operational phase. To speed-up simulation of these models there appears to be a large scope for simplifying them using model-order reduction techniques. In particular we present an example of the use of Proper Orthogonal Decomposition applied to a simple reservoir model for two-phase (oil-water) flow.

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MS2

Structure-preserving Model Reduction for MEMS Modeling

Abstract unavailable at time of publication.

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MS2

Balanced Truncation for Switched Dynamical Systems

A hybrid dynamical system is a system described by both differential equations (continuous flows) and difference equations (discrete transitions). It has the benefit of allowing more flexible modeling of dynamic phenomena, including physical systems with impact such as a bouncing ball, switched systems such as a thermostat, and even internet congestion. Hybrid dynamical systems pose a challenge since almost all reduction methods cannot be directly applied. Here we introduce a balanced truncation-like method for switched linear dynamical systems. For this we define the controllability and observability Gramians for either time-transmission switching or time-invariant switching. For the first case, the Gramians are only the sum of the Gramians of the subsystems, and so the balanced truncated switched system is the sum of the balanced truncated subsystems. For the second case the method is tricky as a notion of uncertainty should be added in order to deal with the special structure of the switched system. We also introduce two new definitions of the Gramians, solutions of either special LMIs or Lyapunov equations to come up with the balanced truncated-like reduced model. With this approach we will preserve the stability for the reduced model. Here one should notice that we supposed implicitly that each subsystem is stable.

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MS2

Interpolatory Projection Methods for Optimal Model Reduction of Large-scale Dynamical Systems

We investigate interpolatory optimal model reduction of large-scale dynamical systems. First, we present a trust-region approach for optimal $\mathcal{H}_\in$ approximation of MIMO systems. The approach generates a sequence of reduced order models producing monotone improving $\mathcal{H}_\in$ error norms and is globally convergent to a reduced order model guaranteed to satisfy first-order optimality conditions. Then, we extend this approach to optimal model reduction of parameterized systems using an $\mathcal{H}_\in \otimes \mathcal{L}_\in$ joint error measure.

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MS2

Stability Issues and DEIM-based Nonlinear Model Reduction

Reduced order model stability is examined for the discrete empirical interpolation based model reduction method (DEIM). A micro-electromechanical and a circuit example are used to demonstrate the stability issue, and stability-enhancing modifications of the algorithm are described. We show that extracting an equilibrium point Jacobian guarantees local DIEM stability, and that multi-point methods for extracting stabilizing projection matrices yields superior global stability. The examples are also used to demonstrate the failure characteristics of DEIM methods.

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MS3

Stochastic and Kinetic Approaches in Mesoscale Modeling of Grain Growth in Polycrystalline Materials

Microstructure evolution is a problem of central importance in materials science. Grain boundary engineering techniques allow to design and manufacture materials predisposed to certain behavior under external conditions. This type of work relies heavily on statistical analysis of grain boundary evolution and of an interplay between micro- and macroscopic properties. We present an account of recent developments in mesoscale theory of texture evolution in polycrystalline materials. The talk will demonstrate how a carefully chosen combination of simulation, theory and modeling techniques can bring a deeper understanding to coarsening processes governed by the motion of triple junctions. By means of modulated stochastic process characterization and kinetic evolution equations, we aim at quantifying the rates of grain boundary disappearance events and predicting the influence of these events on macro-level materials properties. Comparison with large-scale 2D and 3D simulations will provide the necessary validation and reveal similarities and differences between these approaches.

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MS3

Predictive Theory for the Grain Boundary Character Distribution

Most technologically useful materials are polycrystalline microstructures composed of a myriad of small grains separated by grain boundaries. The energetics and connectivity of the grain boundary network plays a crucial role in determining the properties of a material across a wide range of scales. A central problem is to develop technologies capable of producing an arrangement of grains—a texture—that provides for a desired set of material properties. Since the dawn of man, coarsening has been the principal feature of these technologies. Cellular structures coarsen according to a local evolution law, a gradient flow or curvature driven growth, for example, limited by space filling constraints, which give rise to changes in the configuration. There are two aspects of coarsening, geometric growth and texture development. The main objective of this presentation is to show that they may be decoupled and characterized by different types of evolution processes, leading to statistically different types of coarsening rates. We consider the grain boundary character distribution, the GBCD, a basic texture measure, and establish an entropy based theory for it which suggests that GBCD satisfies Fokker-Planck type kinetics. For this, a simplified critical event model is introduced and studied.

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MS3
The Janossy Effect and Hybrid Variational Principles

Light changes the orientation of a liquid crystal. This is the optical Freeder- icksz transition. In the Janossy effect, the threshold intensity for the optical Freedericksz transition is dramatically reduced by the additon of a small amount of dye to the sample. This has been interpreted as an optically pumped orientational rachet mechanism, similar to the rachet mechanism in bi- ological molecular motors and requires an innovative hybrid gradient flow. Joint work with Michal Kowalczyk.

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MS3
Kinetic Theory and Lax Equations for Shock Clustering and Burgers Turbulence

We study shock statistics in scalar conservation laws with random initial data by deriving kinetic equations, which have the form of a Lax pair. This, in addition to some exact solutions to the equation, suggest that the model is a completely integrable system in 2+1 dimensions.

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MS4
People You May Know

Facebook's friend recommendation system helps people connect with their friends. Our system, called People You May Know, uses a combination of results from sociology and machine learning to make the best suggestions possible. We will look at some of the challenges involved in building a system that can handle the scale of Facebook and provide high quality recommendations. In this talk I will discuss both the algorithmic and machine learning challenges that we have faced and overcome in building this system.

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MS4
Modularity and Graph Algorithms

A number of graph partitioning algorithms are based on the concept of modularity. In particular Clauset, Newman and Moore (CNM) have developed a greedy agglomerative graph partitioning algorithm that scales well but is known to have several flaws. Fortunato and Barthelemy have performed a rigorous analysis of the CNM algorithm that elucidates it problems. More recently Berry, Hendrickson, Laviolette, and Phillips have derived a weighted variant of CNM that performs much better in practice. This talk will focus on a different version of the parent CNM algorithm based on a statistical re-interpretation of CNM that also addresses some of the issues with the original algorithm.

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MS4
Scalable Methods for Representing, Characterizing, and Generating Large Graphs

Abstract unavailable at time of publication.

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MS4
Exploiting Sparsity in the Statistical Analysis of Gene Expression Data

Abstract unavailable at time of publication.

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MS5
Multiscale Simulation Techniques for Fluid Structure Interaction

In this talk, I will discuss multiscale simulation techniques for fluid-structure interaction. Our goal is to develop simulation techniques for solving fluid-structure problems with complex microgeometries on a coarse grid. A particular application is fluid flows in deformable fracture porous media. Due to changes in pore pressure, the deformation can significantly alter pore geometry and change permeabilities. Coarse-scale models will be discussed and numerical results will be presented. This is a joint work with Peter Popov, Yuliya Gorb, and Donald Brown.

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MS5

On a Nonlinear Problem Arising in Poroelasticity

In this work we study a model for steady fluid flow in a saturated deformable (elastic) porous medium. The model which was developed in the context of modeling one of the processes in paper production is distinguished in its use of a Kozeny-Carman type relation for the fluid's permeability, resulting in a quasilinear elliptic system. We describe and analyze a finite element method for approximating solutions of this nonlinear problem.

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MS5

Coupling of Elastic and Electromagnetic Waves and Related Mathematical Problems

There are considered theoretical and numerical aspects of the interaction of elastic and electromagnetic waves in complex media. The models considered are different combinations of the Lamé and Maxwell equations. The coupling mechanism is based on the seismomagnetic and electrokinetic effects. Theoretical results of the analytical solution are discussed for various direct and inverse problems. Finally, we give some results of the numerical solution of some direct and inverse problems describing linear processes of interaction of elastic and electromagnetic waves.

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MS5

Fluid Flows in Karst Aquifer

We discuss two types of models for flows in karst aquifer. The first is the coupled Navier-Stokes-Darcy model and its variants. The second is the so-called coupled continuum pipe flow model (CCPF) or conduit flow process model (CFP). Mathematical well-posedness of the models, their numerical approximation, calibration of key physical parameters will be discussed.

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MS6

Nonlinearity and Instability in the Dynamics of Financial Markets

Two recent studies in collaboration with Prof. Caginalp are presented. A large-scale statistical methodology demonstrates a significant role for numerous variables, and extracts key nonlinearities, thereby providing a basis for understanding competing motivations that drive investor decisions. One of the motivations involved is trend, or momentum, a key component of the system of ordinary differential equations modeling price dynamics developed since 1990 (see www.pitt.edu/∼caginalp). We show equilibrium and stability results for this system.

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MS6

The Dynamics of a Durable Consumption Good: Modeling for Experimental Design and Testing

An unprecedented housing bubble, 1997 to 2007 subsequently engulfed the economy from 2007 to the present. Economic theory and experiments have modeled the two polar extremes: (1) Services and other non-durables that perish on consumption, and (2) Durable goods with infinite life. We build on the previous literature to model a simple consumer durable asset, that has a finite expected life, with agent producers who can vary their output of the durable asset depending on its market price and production cost. We characterize the long run stationary equilibrium of the system, and show how it can be combined with existing models of asset pricing to enable the study of short-term dynamic behavior. Part 2.

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MS6

On the Specialization and Division of Exchange, Durability and Market Performance

Robust laboratory studies have long established contrastingly different behavior depending whether the items exchanged are final use goods, with specialized buyers, and sellers, or assets that can be re-traded over multiple periods. The former perform with high efficiency, the latter poorly, tending to bubble and crash. New experiments combine these features in simple markets where durability, and specialization, is varied by imposing or relaxing a restriction on re-trade within each period. Since about 60 percent of national output is consumer non-durable goods and services, a component that resists change in good times or recessions, while economic troubles originate in asset markets, the results illuminate the much greater stability of expenditure patterns in perishable final goods markets relative to durable goods, credit and financial markets.

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MS6

Housing Bubbles and the Economy: Challenge to Modeling

An unprecedented housing bubble, 1997 to 2007 subsequently engulfed the economy from 2007 to the present. Economic theory and experiments have modeled the two polar extremes: (1) Services and other non-durables that perish on consumption, and (2) Durable goods with infinite life. We build on the previous literature to model a simple consumer durable asset, that has a finite expected life, with agent producers who can vary their output of the durable asset depending on its market price and production cost. We characterize the long run stationary equilibrium of the system, and show how it can be combined with existing models of asset pricing to enable the study of short-term dynamic behavior. Part 1.

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MS6

A Profit Keeping and Loss Protection Strategy in Portfolio Management

The widely studied power-utility-maximization strategy is optimal only in the sense of ensemble averaging. However, in reality, only one random path will be realized and the value of the portfolio at the end of the investment horizon could be dramatically lower than its historical high. This is evident in the recent financial crisis. We will present a new strategy to overcome this problem.

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MS7

Positivity-preserving Discontinuous Galerkin Schemes for Linear Vlasov-Boltzmann Transport Equations

We develop a high-order positivity-preserving discontinuous Galerkin (DG) schemes for linear Vlasov-Boltzmann transport equations (BTE) under the action of quadratically confined electrostatic potentials. The solutions of the BTEs are positive probability distribution functions. It is very challenging to have a mass-conservative, high-order accurate scheme that preserves positivity of the numerical solutions in high dimensions. Our work extends the maximum-principle-satisfying scheme for scalar conservation laws by Zhang and Shu (2010) to include the linear Boltzmann collision term. The DG schemes we developed conserve mass and preserve the positivity of the solution without sacrificing accuracy. A discussion of the standard semi-discrete DG schemes for the BTE are included as a foundation for the stability and error estimates for this new scheme. Potential applications of this solver include the modeling of charge transport in nano-scale semiconductor and solar devices and Vlasov-Poisson, Vlasov-Maxwell systems in plasma physics.

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MS7

Topics in Kinetic Simulation: A Brief Look at the Landscape

This talk will be a brief survey of numerical methods used to solve kinetic equations and the current challenges faced by computational scientists in various applications. This includes an overview of topics to be addressed in more detail during the symposium.

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MS7

A Nonlinear Spatial Closure for the 2-D S_n Equations

We present a strictly positive non-linear Petrov-Galerkin method that reduces to the standard linear-discontinuous Galerkin spatial discretization when that method produces a positive solution. In addition to strictly positive angular flux solutions, our method offers preservation of the P_1 spatial moments of the transport equation. Computational results for several test problems in both slab and rectangular geometries are presented.

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MS7

Conservative High Order Semi-Lagrangian Finite Difference Weno Methods for Advection in Incompressible Flow and Kinetic Equations

We propose a novel semi-Lagrangian finite difference formulation for approximating conservative form of advection equations with general variable coefficients. Compared with the traditional semi-Lagrangian finite difference schemes, which are designed by approximating the advective form of equation via direct characteristics tracing, the scheme we proposed approximates the conservative form of equation. This essential difference makes the proposed scheme conservative by nature, and extendable to equations with variable coefficients. The proposed semi-Lagrangian finite difference framework is coupled with high order essentially non-oscillatory (ENO) or weighted ENO (WENO) reconstructions to achieve high order accuracy in smooth parts of the solution and capture sharp interfaces without introducing oscillations. The scheme is extended to high dimensional problem by Strang splitting. The performance of the proposed schemes is demonstrated by linear advection, several challenging examples of rigid body rotation and swirling deformation in multi-dimensions. As the information is propagating along characteristics, the semi-Lagrangian scheme does not have CFL time step restriction, allowing for a cheaper and more flexible numerical realization than the regular finite difference scheme for some problems.

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MS8

Anchor Point in ANOVA Decomposition with Applications to Stochastic Problems

Analysis of variance (ANOVA) is presented to lift the curse of dimensionality for high dimensional problems. We focus on anchored-ANOVA representation employing the Dirac measure that converges exponentially for certain classes of functions. However, the error depends on the anchor points. We investigate which anchor points give the best approximation. We then present examples of a function approximation as well as numerical solutions of the stochastic advection equation using a combination of anchored-ANOVA and polynomial chaos expansions.

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MS8

A Sparse Approximation of Partial Differential Equations with Random Inputs

In this work, using techniques based on *concentration of measure theory* we derive a method for approximation of sparse solution of stochastic PDEs. The proposed method is:

- Non-intrusive: It is based on the direct solution sampling,
- Provably convergent: We obtain probabilistic bounds on the approximation error proving the convergence of the method,
- Well suited for high dimensional problems.

Several numerical experiments will be presented to explore different aspects of the proposed method.

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MS8

Stochastic Collocation Methods on Arbitrary Nodes

We present a stochastic collocation strategy based on multivariate interpolation theory. The key feature of the method is that it allows simulations on collocation nodes (sampling points) of arbitrary number and at arbitrary locations in arbitrary dimensional spaces. Therefore the method results in great flexibility for practical stochastic simulations, particularly in high dimensions. We present mathematical analysis on the well-posedness and properties of the method, as well as numerical examples illustrating its high-order convergence properties.

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MS8

A Stochastic Heterogeneous Multiscale Method for Porous Media Flow

Abstract not available at time of publication.

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MS9

Krylov Subspace Enhanced Parareal Algorithms

We are interested in a variant of the parareal algorithm introduced by Farhat et al., which uses previous iterations in order to create a subspace in which a more accurate coarse approximation of the solution is sought at each iteration. We show that this approach can be interpreted as a Krylov subspace method with an incomplete subspace: there are missing powers of the iteration matrix. This leads to a new and interesting polynomial approximation problem.

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MS9

Parallel Deferred Corrections and Parareal

A method for temporal parallelization which combines features of the parareal algorithm and spectral deferred correction methods will be presented. This approach can be viewed either as a way to parallelize deferred corrections, or as a technique for improving the efficiency of the parareal algorithm.

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MS9
Parallel Implicit Deferred Corrections

We present an extension of revisionist integral deferred correction, a parallel high order time integrator, to solve stiff systems implicitly. Based on the corrector-predictor model, the main idea is to decouple the prediction and correction steps so that they can be run in parallel. Time permitting, we apply our algorithms to stiff rate equations.

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MS9
A Parallel in Time Solver for Optimal Control Problems

In this talk, we present a general methodology that couples optimization algorithms and time parallelization techniques to tackle optimal control issues. Our approach consists in defining two sets of N initial intermediate values and N intermediate targets, so that the initial problem is split into N independent smaller problems. To illustrate the efficiency of our strategy, we apply it to quantum (bilinear) control setting and to the control of parabolic equation.

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MS10
Random Vectors, Random Matrices, and Diagrammatic Fun

If x, y, and z are random vectors, what is the expectation of the product of their inner products, $< x, y >< y, z >< z, x >$? If U and V are random unitary matrices, what is the expected trace of their commutator? Diagrammatic methods for evaluating integrals like these, which transform them into combinatorial problems, are starting to show up in computer science. I will describe two applications: showing that a simple "product of inner products" function of directed graphs is #P-complete, and showing that certain estimators for the permanent, based on determinants over nonabelian algebras, have exponentially large variance. This is joint work with Alex Russell.

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MS10
Discrete Models of Colloids

Colloids are mixtures of substances that tend to separate so that like particles are clustered together. Unlike related models with enthalpic forces causing like particles to attract or disparate particles to repel, colloids are driven solely by entropic forces. It seems that in these models clustering occurs above a certain density if configurations are chosen from the uniform distribution. The challenge in studying colloids is that there are very few rigorous results and it even appears difficult to efficiently simulate these systems to test hypotheses experimentally. We study several discrete models of colloids with large squares suspended in a sea of small diamonds and rigorously show that the squares will cluster together beyond a certain density, extending a result of Frenkel and Louis. We also study heuristics due to Buhat, Dress and Krauth for sampling configurations of colloids and show that their algorithms are provably efficient in certain settings and inefficient in others. (This is joint work with Sarah Miracle and Amanda Pascoe.)

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MS10
Phase Transitions for Random Graph Processes

The classic random graph evolution of Paul Erdős and Alfred Rényi undergoes a phase transition. Parametrizing the number of edges as $t\frac{n}{2}$ there is a critical point $t_{cr} = 1$. For $t < t_{cr}$ all components are small while when $t > t_{cr}$ a "giant component" has emerged. The Bohman-Frieze process places more weight on joining isolated vertices. We define the susceptibility of a graph, give a differential equation for its value, and and show that t_{cr} is that t at which the value explodes. We examine the fine behavior near criticality, particularly the growth of the "baby giant" at $t_{cr} + \epsilon$. We discuss other processes, including the Product Rule process for which simulations indicate very different behavior near criticality. (Joint work with Svante Janson, Milyun Kang, Will Perkins and others.)

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MS10
Spectral Sparsification of Graphs

A sparsifier of a graph G is a sparse graph that is a good approximation of G. We consider the problem induced by measuring quality of approximation in a spectral sense. We describe deterministic polynomial-time algorithms that produce excellent sparsifiers, and fast randomized algorithms that produce cruder sparsifiers.

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MS11
Subdomain Radial Basis Collocation Method for Fracture Mechanics

This work attempts to apply radial basis collocation method to fracture mechanics by introducing a domain decomposition technique with proper interface conditions. The proposed method allows (1) natural representation of discontinuity across the crack surfaces and (2) enrichment of crack-tip solution in a local subdomain. Exponential convergence rate can be achieved while keeping the discrete system well-conditioned. The analytical prediction and numerical results demonstrate that an optimal dimension of the near-tip subdomain exists.

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MS11
The Gibbs Phenomenon for Radial Basis Functions

The Gibbs phenomenon was first observed in the context of truncated Fourier expansions, but it arises also in cases such as truncated integral transforms and different interpolation methods. Radial basis functions (RBFs) include both splines and trigonometric interpolation as special cases in 1-D, and they generalize these methodologies to scattered node layouts in any number of dimensions. We investigate here the Gibbs phenomenon in the case of RBF interpolation on an equispaced grid in 1-D.

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MS11
An RBF-Gegenbauer Method for Time Dependent Discontinuous Problems

Radial basis function(RBF) methods have been actively developed in the last decades. The advantages of RBF methods are that these methods are mesh-free and yield high order accuracy if the function is smooth enough. The RBF approximation for discontinuous problems, however, deteriorates its high order accuracy due to the Gibbs phenomenon. In this talk we will show that high order accuracy can be recovered from the RBF approximation contaminated with the Gibbs phenomenon if a proper reconstruction method is applied. In this work, the Gegenbauer reconstruction method is used to reconstruct the RBF approximation for the recovery of high order accuracy. Numerical examples including the linear and nonlinear hyperbolic partial differential equations are presented.

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MS11
Meshfree Solutions of One-dimensional Inviscid Euler Equations

The inviscid Euler equations are solved by expanding any dependent variable in terms of radial basis functions and time dependent expansion coefficients. Using rotational and translational transformations, the Euler equations are solved as exact time dependent differential equations in a moving frame. Riemann solvers are used to calculate various wave interactions. The eigenvalues of the time amplification matrix are all unity. No artificial viscosity, upwinding or entropy violating methods were needed.

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MS12
On the Stochastic Navier-Stokes Equations

Abstract unavailable at time of publication.

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MS12
Filter Based Stabilization for Evolution Equations

This project, which describes joint work with Vince Ervin (Clemson) and Monika Neda (UNLV), considers the following idea: Step 1: Take one step of any numerical method for advancing an evolution equation in time, Step 2: take the result of Step 1, Filter it and use that for the following step. We show how this process Evolve then Filter can overdiffuse an approximate solution. We then show how to fix it to produce a highly accurate, stable and non-overdiffused approximation. One advantage of this approach to stabilization is that Steps 1 and 2 can be performed by calls to independent, black box programs.

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MS12
Analysis of Generalized Alpha-models of Turbulence

In this talk I will discuss the global existence and uniqueness results for the general family of regularized Navier-Stokes and Magnetohydrodynamics (MHD) models . This family captures most of the specific regularized models that have been proposed and analyzed in the literature, including the Navier-Stokes equations, the Navier-Stokes-α model, the Leray-α model, the Modified Leray-α model, the Simplified Bardina model, the Navier-Stokes-Voight model, the Navier-Stokes-α-like models, and certain MHD models, in addition to representing a larger 3-parameter family of models not previously analyzed. We give a unified analysis of the entire three-parameter family of models using only abstract mapping properties of the principal dissipation and smoothing operators, and then use assumptions about the specific form of the parameterizations, leading to specific models, only when necessary to obtain the sharpest results.

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MS12

Drag and Lift Computations of High Order Accuracy Fluid Flow Models

Numerical studies based on finite element discretizations of a higher order time relaxation models of fluid motion will be presented. The family of models is based on filtering and deconvolution techniques for driving the unresolved fluctuations to zero. Optimal error estimates for velocity convergence analysis are derived. The family of models is tested on a benchmark problem where drag and lift estimates and pressure drop on a body immersed in a fluid were investigated.

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MS12

Solving the Navier-Stokes Equations for Velocity, Vorticity and Helicity

For the three-dimensional incompressible Navier-Stokes equations, we present a formulation featuring velocity, vorticity and helical density as independent variables. We show that mathematically the helical density can be observed as a Lagrange multiplier corresponding to the divergence-free constraint on the vorticity variable. As one possible practical application of this formulation, we consider a time-splitting numerical scheme based on a simple alternating procedure between vorticity - helical density and velocity - Bernoulli pressure systems of equations. We discuss the relation of the numerical method to some well known turbulence models.

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MS13

High Order Accurate Discretization of the Wave Equation on Structured Grids

Enforcement of boundary conditions in high-order embedded-boundary methods that removes small-cell stiffness for both Dirichlet and Neumann b.c. and guarantee single valued solutions for slender bodies is presented. The b.c. enforcement is paired with Taylor-series-time-stepping and a high-order spatial discretization to accurately solve the wave equation. Three spatial discretizations are considered: Pade (implicit), summation by parts finite difference and Fourier continuation. Numerical experiments illustrating the properties of the methods are presented.

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MS13

Complete Radiation Boundary Conditions: Theory and Application

Complete radiation boundary conditions (CRBCs) are geometrically flexible, applicable to all standard wave equations in homogeneous, isotropic media as well as to a limited class of anisotropic models, and satisfy optimal complexity estimates. They provide provably accurate long-time results on small domains using parameters which are determinable a priori. We review the CRBC theory and describe our ongoing efforts to develop a generally usable implementation and to extend their applicability to more complex models.

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MS13

Stable Fourier Based Embedding Methods for Wave Propagation on Complex Domains

The FC-AD methodology provides efficient new PDE solvers based on the use of a certain "Fourier continuation' (FC) method in conjunction with alternating direction (AD) strategies and can be applied directly to complex computational domains with unconditional stability and high-order accuracy. FC-AD techniques are uniquely suited for wave propagation problems as the Fourier basis essentially eliminates pollution error. New extensions including those to handle Neumann- and mixed-type boundary conditions will be presented.

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MS13

Boundary and Interface Conditions for Non-Linear Wave Propagation Problems

Most wave propagation problems are linear and the related boundary and interface conditions that lead to well-posedness and stability are relatively well known. For non-linear problems that is not the case. We will discuss boundary treatments where the non-linearity adds additional complications. Typical applications that will be disussed are related to shocks in fluid flow, propagation of discontinuities in stochastic PDE's and earthquake problems.

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MS14

Randomization in the Default Boundary Problem

We consider an inverse problem for the first hitting time distribution of a Wiener process and its application for credit risk pricing. We demonstrate that randomization of the initial state of the process lead to analytically tractable solution.

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MS14

Modeling Default Correlation and Clustering: A Time Change Approach

We present a novel framework for modeling correlated defaults where it is possible to capture the so-called "contagion effect'. Time changing multi-parameter Markov processes with multivariate subordinators leads to jump-diffusion processes that are correlated through their jump measures. When unpredictable shocks arrive, the default intensity of multiple firms will shift simultaneously, which can trigger multiple defaults.

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MS14

Pricing Counterpary Risk at the Trade Level and CVA Allocation

We address the problem of allocating the counterparty-level credit valuation adjustment (CVA) to the individual trades composing the portfolio. We show that this problem can be reduced to calculating contributions of the trades to the counterparty-level expected exposure (EE) conditional on the counterparty's default. We propose a methodology for calculating conditional EE contributions for both collateralized and non-collateralized counterparties. Calculation of EE contributions can be easily incorporated into exposure simulation processes that already exist in a financial institution. We also derive closed-form expressions for EE contributions under the assumption that trade values are normally distributed. Analytical results are obtained for the case when the trade values and the counterparty's credit quality are independent as well as when there is a dependence between them (wrong-way risk).

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MS14

Pricing Structured Credit Products with Implied Factor Models

The current financial crisis has underscored the need for transparent and robust methods for valuing and hedging structured credit portfolios. First-generation models, such as the Gaussian copula-based methods have well documented practical and theoretical limitations. In this paper, we demonstrate the practical application of the weighted Monte Carlo methodology to value and compute sensitivities and risk statistics for ABS and CLO structures. The model extends the full bottom-up approach of Rosen and Saunders (2009) for pricing bespoke CDOs to include cancellability and stochastic LGDs in a natural way. The performance of the model is analyzed throughout a three-month period during the credit crisis in 2008. The model calibrates very well to observed prices for the CDXHY and LCDX indices, and provides stable implied distributions for the systematic factor. Furthermore, it gives robust, consistent prices and sensitivities , even during this very volatile period.

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MS15

Linear Feedback Control Strategies for the Navier-Stokes Equations

One systematic control strategy often proposed for fluid flows is optimal feedback control of the linearized system. If the linearized portion of the Navier-Stokes equations are stabilized, then the full nonlinear system is stabilized. The natural questions are practical-how does this strategy perform in practice. This talk will focus on a numerical procedure for solving the LQR control problem associated with the Oseen equations and numerical experiments to determine the effectiveness of the feedback control strategy.

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MS15

Bridging the Boussinesq and Primitive Equations Through Spatio-Temporal Filtering

We propose a novel approach for bridging the Boussinesq equations and the primitive equations. This approach uses spatio-temporal filtering as an alternative to traditional scaling arguments used in the derivation of simplified models for the ocean and atmosphere.

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MS15

Improving Mass Conservation in FE Computations of NSE with C0 Velocities

This talk will begin by introducing the Scott-Vogelius element pair, then show a connection between it and the grad-div stabilized Taylor-Hood element. Implications of this connection will be discussed, and numerical experiments will also be given.

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MS15

Two-Level Strategies for Large Eddy Simulation Proper Orthogonal Decomposition Models

One of the main hurdles in the development of modern closure models in Proper Orthogonal Decomposition of turbulent flows has been the lack of efficient computational strategies for the discretization of the associated nonlinearities. We introduce a two-level discretization methodology that reduces dramatically the computational cost without compromising the accuracy of the closure model. This is demonstrated numerically in the 3D simulation of a flow past a cylinder at Re=1,000.

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MS16

Collective Behavior of Two Classes of Car Following Models

In this talk I'll focus on fundamental properties of two specific car-following (CF) models of highway traffic; namely he Intelligent Driver Model, IDM, and the Aw-Rascle-Greenberg Model, ARG. I shall show that for both of these models there are no car crashes and no velocity reversals. These results concern well-posedness of the underlying ODE system and are addressed by a-priori estimates which are independent of the number of cars in the system. I shall also establish that both the IDM and ARG models support large amplitude Stop and Go waves; these waves are traveling wave solutions of the underlying systems.

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MS16

Impact of Protein and Lipid Binding on Drug Disposition

Abstract unavailable at time of publication.

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MS16

Solutions of Semilinear Equations

We study solutions of a second order semilinear pde, with particular focus on singular solutions. For both the focussing and non-focussing versions of the equation we find new singular solutions.

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MS16

A Weak KAM Theorem for the Nonlinear Vlasov System

The space $L^2(0,1)$ has a natural Riemannian structure on the basis of which we introduce an $L^2(0,1)$–infinite dimensional torus **T**. For a class of Hamiltonians defined on its cotangent bundle we establish existence of a viscosity solution for the *cell problem* on **T** or, equivalently, we prove a Weak KAM theorem. As an application, we obtain existence of absolute action-minimizing solutions of prescribed rotation number for the one-dimensional nonlinear Vlasov system with periodic potential.

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MS17

Practical Heuristics for Inexact Subgraph Isomor-

phism

Abstract unavailable at time of publication.

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MS17
Spectral Methods for Subgraph Detection

We describe a statistical test for subgraph detection and localization using spectral properties of the so-called modularity matrix, a type of residual under the Chung-Lu random graph model. We show that the resultant algorithmic procedure can be applied to very large graphs ($< 10^6$ vertices), with complexity dominated by that of standard sparse eigensolver methods, and can successfully isolate anomalous vertices in real data examples.

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MS17
Tools and Primitives for High-performance Graph Computation

Abstract unavailable at time of publication.

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MS17
Hybrid Parallel Programming for Massive Graph Analysis

Abstract unavailable at time of publication.

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MS18
Deciding to Give Up Tenure: Surprising Decisions Along the Path

In a world where a successful research program and tenure often seem to be the main goals of a Ph.D. scientist, one may find it hard to see the other options available. After receiving my degree, my choices were not unusual and I spent three years as a postdoc before accepting a tenure-track position and, later, receiving tenure. But life sometimes throws unexpected opportunities in your path and I will describe a number of my own experiences, including how I eventually reached a decision to resign a tenured position.

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MS18
Taking the Road Not [Usually] Taken

There are commonalities among research career paths; however, internally motivated and externally mandated transitions help mold each experience into our own unique journey. I will discuss major transition points in my professional career ranging from graduate school to early career and personal as well as externally motivated events that brought me to career crossroads. My experience and possible lessons learned in taking less traveled paths will be examined.

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MS18
Panel Discussion: Success through Transitions

This panel session provides an opportunity for AWM workshop members to ask questions and discuss issues with professional development speakers.

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MS18
Title Not Available at Time of Publication

Abstract unavailable at time of publication.

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MS19
FETI Methods for Mortar Coupling of Stokes-Darcy Systems

Abstract unavailable at time of publication.

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MS19
An Efficient Method for Solving Multiscale Elliptic Problems with Randomly Perturbed Data

We propose a method for efficient solution of elliptic problems with multiscale features and randomly perturbed coefficients. We use the multiscale finite element method (MsFEM) as a starting point and derive an algorithm for solving a large number of problems with randomly perturbed coefficients. We show that the method converges to the multiscale finite element solution in the limit. A set of numerical examples is presented to illustrate theoretical

findings.

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MS19

Some Computational Issues in the Modeling and Simulation of Coupled Surface and Subsurface Fluid Flow

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MS20

Adaptive Strategies for Uncertain Hyperbolic Systems

Abstract not available at time of publication.

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MS20

A Multi-element Probabilistic Collocation Based Kalman Filter for Power System Dynamic State Estimation

In this talk, we propose an efficient multi-element probabilistic collocation method (MEPCM) based Kalman filter (KF) to include dynamic state variables in the power system dynamic state estimation process. Comparing with Monte Carlo (MC) based KF approach, the proposed MEPCM based KF implementation can solve the system of stochastic state equations much more efficient. Additionally, the proposed approach can sample the generalized polynomial chaos approximation of the stochastic solution with an arbitrarily large number of samples, at virtually no additional computational cost. The proposed algorithm thus can drastically reduce the sampling errors and achieve a high accuracy at reduced computational cost, compared to the classical MC implementations of KF. The proposed MEPCM-KF based dynamic state estimation is tested on both single-machine and multi-machine system with various random disturbances. Our numerical results demonstrate the validity and performance of the proposed dynamic state estimation approach with different random disturbance. The numerical results also indicate the proposed approach can include the full dynamics of power systems and ensure an accurate representation of the changing states in the power system.

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MS20

Capturing All Scales of Random Modes in Stochastic Pdes Based on Polynomial Chaos and a Dynamically Adaptive Wavelet Method

We consider the numerical solution of stochastic partial differential equations based on polynomial chaos expansion exemplified by the convection-diffusion equation model. This typically produces a coupled system of deterministic equations for the coefficients of the expansion whose size can become very large with an increasing number of independent random variables and/or order of polynomial chaos expansion (dubbed the dimensionality curse). We tackle this challenge using a dynamically adaptive wavelet-based methodology utilizing space-refinement that allows capturing all scales of each random/unceretainty mode on indepenent grids. We present numerical results illustrating the salient features of the proposed method.

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MS20

Multi-element Uncertainty Quantification Based on Simplex Elements Stochastic Collocation

A Simplex Elements Stochastic Collocation (SESC) method is presented for robust and efficient multi-element uncertainty quantification. The method is equally robust as Monte Carlo simulation in terms of the Extremum Diminishing (ED) robustness concept extended to probability space. Its efficient extension to multiple uncertainties is considered based on higher degree polynomial interpolation, randomized refinement sampling, and Essentially Extremum Diminishing (EED) extrapolation. These strategies employ the flexibility of simplex elements for handling randomized samples and non-hypercube probability spaces.

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MS21

Anatomy of a Young Giant Component in the Random Graph

In this talk, we will completely describe the structures of giant components in random graphs $G(n,p)$ with $n^{-1/3} << pn-1 << n^{-1/4}$. The description can be made by using random 3-regular graphs and Galton-Watson Poisson branching processes. The proof uses the Poisson cloning model and interesting computation arguments. We will also present some results regarding the diameter and the mixing time of the giant component.

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MS21

How Frequently is a System of 2-linear Boolean Equations Solvable?

We consider a random system of equations $x_i + x_j = b_{(i,j)}(\mathrm{mod}2)$, $(x_u \in \{0,1\}, b_{(u,v)} = b_{(v,u)} \in \{0,1\})$, with the pairs (i,j) from E, a symmetric subset of $[n] \times [n]$. E is chosen uniformly at random among all such subsets of a given cardinality m; alternatively $(i,j) \in E$ with a given probability p, independently of all other pairs. Also, given E, $Pr\{b_e = 0\} = Pr\{b_e = 1\}$ for each $e \in E$, independently of all other $b_{e'}$. It is well known that, as m passes through $n/2$ (p passes through $1/n$, resp.), the underlying random graph $G(n, \#\text{edges} = m)$, ($G(n, Pr(\text{edge}) = p)$, resp.) undergoes a rapid transition, from essentially a forest of many small trees to a graph with one large, multicyclic, component in a sea of small tree components. We should expect then that the solvability probability decreases precipitously in the vicinity of $m \sim n/2$ ($p \sim 1/n$), and indeed this probability is of order $(1-2m/n)^{1/4}$, for $m < n/2$ ($(1-pn)^{1/4}$, for $p < 1/n$, resp.). We show that in a near-critical phase $m = (n/2)(1+\lambda n^{-1/3})$ ($p = (1+\lambda n^{-1/3})/n$, resp.), $\lambda = o(n^{1/12})$, the system is solvable with probability asymptotic to $c(\lambda)n^{-1/12}$, for some explicit function $c(\lambda) > 0$. Mike Molloy noticed that the Boolean system with $b_e \equiv 1$ is solvable iff the underlying graph is 2-colorable, and asked whether this connection might be used to determine an order of probability of 2-colorability in the near-critical case. We answer Mike's question affirmatively and show that probability of 2-colorability is $\lesssim 2^{-1/4}e^{1/8}c(\lambda)n^{-1/12}$, and asymptotic to $2^{-1/4}e^{1/8}c(\lambda)n^{-1/12}$ at a critical phase $\lambda = O(1)$, and for $\lambda \to -\infty$. In part, this study was inspired by the work of Hervé Daudé and Vlady Ravelomanana who analyzed the case of a random *multigraph* $MG(n, \#\text{edges} = m)$. This is a joint work with Dr. Ji-A Yeum.

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MS21

Structure of Random r-SAT below the Pure Literal Threshold

It is well known that there is a sharp density threshold for a random r-SAT formula to be resolved by the pure literal rule, and a higher threshold for satisfiability. We analyze the structure of the (rare) unsatisfiable instances below the pure literal threshold, contrasting this with the situation above the satisfiability threshold. It remains open what happens between the two thresholds.

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MS21

Phase Transition for the Mixing Time of the Glauber Dynamics for Coloring Regular Trees

We prove that the mixing time of the Glauber dynamics for random k-colorings of the complete tree with branching factor b undergoes a phase transition at $k = b(1 + o_b(1))/\ln b$. Our main result shows nearly sharp bounds on the mixing time of the dynamics on the complete tree with n vertices for $k = Cb/\ln b$ colors with constant C. For $C \geq 1$ we prove the mixing time is $O(n^{1+o_b(1)}\ln^2 n)$. On the other side, for $C < 1$ the mixing time experiences a slowing down, in particular, we prove it is $O(n^{1/C+o_b(1)}\ln^2 n)$ and $\Omega(n^{1/C-o_b(1)})$. The critical point C=1 is interesting since it coincides (at least up to first order) to the so-called reconstruction threshold which was recently established by Sly. The reconstruction threshold has been of considerable interest recently since it appears to have close connections to the efficiency of certain local algorithms, and this work was inspired by our attempt to understand these connections in this particular setting. This is joint work with Prasad Tetali, Juan C. Vera, and Linji Yang which appeared at SODA'10.

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MS22

Radial Basis Function Methods for Delayed Equations with Discontinuities

An adaptive meshless numerical scheme for the solution of neutral- and delayed differential equations based on multiquadrics (MQ) collocation is presented. Furthermore, we report on our progress to extend the method to deal with state-dependent neutral differential equations. This kind of nonlinear problem may be numerically elusive due to its ability to form and propagate discontinuities and low-order singularities in the solution, which may take place at times not known in advance. The ultimate goal is to infer the singularity locations in computing time by monitoring the MQ weights in the interpolant and then partition the time domain into smooth subintervals.

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MS22

Anti-Gibbs and Anti-Runge Strategies in Spectral Methods

We discuss the relationship between the Gibbs and Runge Phenomena and compare and contrast single-interval and three-interval strategies for combating them. RBF, Fourier and polynomial bases are analyzed. The limitations of these tactics in both accuracy and ill-conditioning and the trade-offs are discussed.

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MS22

Kernel-based Approximation for Ill-posed and Discontinuous Problems

In this talk we present the idea of meshless computational methods based on the use of kernel-based functions for solving various ill-posed problems and problems with discontinuity. In particular, the recent development of the method of fundamental solutions combined with various regularization techniques to solve Cauchy problems and inverse heat conduction/source identification problems will be discussed. The main idea is to approximate the unknown solution by a linear combination of fundamental solutions whose singularities are located outside the solution domain. More recent works on using the particular solutions and Green's functions will be highlighted.

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MS22

Detecting Edges in Two Dimensional Functions with Radial Basis Functions

We extend the iterative adaptive multiquadric radial basis function (RBF) method for the detection of local jump discontinuities in one-dimensional problems to two-dimensional problems. The iterative edge detection method is based on the observations that the absolute values of the expansion coefficients of RBF approximation have different growth rates. We consider two approaches: the dimension-by-dimension technique and the global extension approach. Numerical examples demonstrate that the two-dimensional iterative adaptive RBF method yields accurate results.

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MS23

Regulatory Network Analysis and Approximation Using Tensor Products

We consider the problem of recovering a system of functions governing a regulatory network using time course data, such as that obtained from microarrays. The number of components in the regulatory networks and the cost of data collection yield an ugly showing of the curse of dimensionality. In [Gregory Beylkin, Jochen Garcke, and Martin J. Mohlenkamp. 'Multivariate regression and Machine Learning with Sums of Separable Functions," SIAM Journal on Scientific Computing (2009)] it was shown that regression with tensor products provides a way to effectively overcome this and obtain good approximations. We will incorporate time derivatives into a novel ALS algorithm for approximating time course data. We will then consider the benefits of using tensor product in the analysis of the approximated network.

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MS23

Solution of High-Dimensional Uncertain Systems Using Separated Tensor Decomposition

Separated representations have proven efficient to relax the curse-of-dimensionality associated with approximation of high-dimensional functions and tensors. In this talk, we will demonstrate how such techniques can be employed to efficiently compute the solution to linear elliptic PDEs with high-dimensional random inputs. In particular, we illustrate the existence of an approximate low-rank separated solution to this class of stochastic PDEs and further explore the efficiency and accuracy of alternating least-squares and Rayleigh-Ritz methods in computing the solution.

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MS23

Source Apportionment of Particulate Matter Based on Segregated Composition Size Data

Source apportionment on bulk airborne particle composition data resolves the data into a product of two matrices, source profiles and source contributions. However, size-segregated data requires a higher dimension model since source emissions are size dependent. Source profiles are a composition matrix as a function of size. The model sums outer products of matrices times vectors. The application of this model to data collected using a multiple stage DRUM impactor analyzed by synchrotron XRF will be presented.

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MS23

Convergence Results of a Regularized Tensor Alternating Least-Squares

The Alternating Least-Squares (ALS) for tensor decomposition has been widely applied to many applications, for example, in signal processing, chemometrics, and data mining. However, ALS can be prohibitively slow for some data. We improved ALS with a regularization term. Our regularized method dramatically accelerates ALS. In addition to providing numerical results for several data sets, we also analyze the convergence of the regularized ALS.

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MS24

Diffeomorphic Deformation of Textured Shapes

This work proposes a new method to match shapes with interior textures through the large deformation diffeomorphic metric mapping, resulting in optimizing for geodesics on the space of diffeomorphisms connecting textured shapes. This study is to address the problems caused by boundary conditions and response to the need of matching regions of interest directly in medical applications. The new method is illustrated by numerical experiments on MRI images.

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MS24

Discontinuous Galerkin Solvers for Boltzmann-Poisson Systems in Semiconductor Device Simulations

The Boltzmann transport equation (BTE) is an integro-differential model describing the evolution of a single point probability distribution function. The mathematical and computational difficulties associated to this equation is due to the balance of a first order transport term to an integral operator accounting for their interactions and the coupling to the Poisson equation. We will present a discontinuous Galerkin solver for the Boltzmann Poisson systems. We have implemented this scheme to model hot electron-hole transport on Kane and full energy bands in the simulation of one and two-physical and three-phase space dimensional nano meter devices with a base channels of the order of 50 nm. The energy bands (conduction and valence) are computed by eingenvalue solvers for electronic structures and coupled to the Boltzmann Poisson solver.

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MS24

New Models of Chemotaxis: Analysis and Numerics

Patlak-Keller-Segel (PKS) system is a classical PDE model of the chemotaxis. The system admits solutions that develop delta-type singularities within a finite time. Even though such blowing up solutions model a concentration phenomenon, they are not realistic since biological cells do not converge to one point (while the cell density grows sharply, it must remain bounded at all times). I will present a new chemotaxis model, which can be viewed as a regularized PKS system. The proposed regularization is based on a basic physical principle: boundedness of the chemotactic convective flux, which should depend on the gradient of the chemoattractant concentration in a nonlinear way. Solutions of the new system may develop spiky structures that model the concentration phenomenon. However, both cell density and chemotattractant concentration remain bounded. The proposed model is studied both analytically and numerically. I will first prove a global existence result and then use the bifurcation theory to investigate existence of nontrivial steady states and their stability properties. Finally, I will persent one- and two-dimensional numerical examples that support the analytical findings and demonstrate the formation and stability of the spiky solutions.

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MS24
Well-Balanced Positivity Preserving Central-Upwind Scheme on Triangular Grids for the Saint-Venant System

We introduce a new second-order central-upwind scheme for the Saint-Venant system of shallow water equations on triangular grids. We prove that the scheme both preserves stationary steady states (lake at rest) and guarantees the positivity of the computed fluid depth. Moreover, it can be applied to models with discontinuous bottom topography and irregular channel widths. We demonstrate these features of the new scheme, as well as its high resolution and robustness in a number of numerical examples.

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MS24
Stencil Choosing Sensitivity in WENO

The weighted essentially non-oscillatory method is used to approximate the numerical flux in hyperbolic PDEs. It automatically centers the stencil in the case of a smooth solution, but places larger weights on the smoother stencils when the solution has a discontinuity pr sharp gradient. A significant parameter in determining the WENO weights, epsilon, is examined in this talk.

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MS25
Mathematical and Computational Techniques for Modeling Heavy Oil Reservoirs

While mathematical modeling has been successful in the recovery of conventional oil, it is still in the early stage of heavy oil modeling. As conventional oil reserves dwindle and oil prices rise, heavy oil is now the center stage. Enhanced heavy oil recovery methods are an intensive research area in the oil industry, and have recently generated a battery of recovery methods in what is the largest growing sector of this industry, such as steam assisted gravity drainage (SAGD) and cyclic steam stimulation (CSS). However, the environmental impacts of these processes and the use of a high volume of water and natural gas suggest that extensive research is required for economic and environmentally friendly development of heavy oil reserves. This presentation will give an overview on current research in heavy oil modeling, and the presenter will also describe his current research program.

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MS25
Rate and Interfacial Tension Dependent CO2 Relative Permeability

We must develop models that better quantify and predict the influence of important processes and small-scale features on fluid behavior and CO2 containment potential. Recent relative permeability experiments indicate the dependency of supercritical CO2 on interfacial tension as results of changes in insitu pressure and temperature. We investigate the roles of capillary and gravitational forces on trapped CO2 taking into the account the density, viscosity, and interfacial tension computed from the compositional phase behavior model. The combined capillary number and bond number referred to as trapping number is successfully implemented in IPARS simulator. Carbon storage simulation results with this new modeling capability will be presented.

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MS25
Towards Accurate and Efficient Computational Modeling of Compositional Multi-Phase Flow

Compositional multiphase flow modeling is demanded in a number of important reservoir applications. One important application is the injection of CO_2 in hydrocarbon reservoirs, which is becoming increasingly attractive due to issues related to global warming, and urgent need for improved hydrocarbon recovery. CO_2 injection may be one of the most attractive options for water-flooded reservoirs either from natural water drive or from external water injection. Coinjection of water with CO_2 for improved mobility and increased sweep is also another process of high interest. To evaluate the efficiency of CO_2 injection in water-flooded reservoirs, three-phase compositional numerical models are required. Such simulators have to be equipped with unique capabilities due to special features of CO_2 mixing in hydrocarbon liquids and gases for CO_2 applications. Specifically, when dissolved in liquids, CO_2 generally increases the density. The density increase may have a significant effect on flow path and may result in convective mixing. Moreover, CO_2 mixing may also lower the viscosity; it may also increase the viscosity when there is substantial vaporization of liquid components in the gas phase. In this talk, we present three-phase compositional flow using higher-order finite element methods. Our numerical model is based on an iterative IMPEC coupling of the pressure equation and species transport equations, which are solved by mixed finite element (MFE) and discontinuous Galerkin (DG) methods, respectively. Compared with lower order finite volume methods, the proposed MFE-DG method has low numerical diffusion and can capture the solution discontinuities and yield accurate prediction of shock locations arising in computational three-phase flow.

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MS25
Compositional Flow Modeling in Porous Media

Abstract unavailable at time of publication.

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MS26
Methods and Extensions for Parametric Inference

In computational biology, many dynamic programming algorithms can be interpreted as sum-product algorithms. Examples include Needleman–Wunsch and Viterbi algorithms. Equivalently, these algorithms find the leading term of a given multivariate polynomial F presented by a short and structured factorization. The term-order is part of the input to the sum-product algorithm – and usually depends on biological parameters which are estimated or guessed. Given this unavoidable uncertainty in the term-order, it is desirable to compute all leading terms of F under all term-orders – or equivalently, compute the Newton polytope $NP(F)$. This is called parametric inference. In this talk, we discuss a general framework for parametric inference, and review existing results. Then, motivated by biological applications, we propose two key extensions: 1) parametric k-best inference, and 2) constrained parametric inference. We finish by presenting recent results for these extensions.

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MS26
Hermite Polynomial Aliasing

A representation of Hermite polynomials of degree $2n + 1$, as sum of an element in the polynomial ideal generated by the roots of the Hermite polynomial of degree n and of a reminder, suggests a folding of multivariate polynomials over a finite set of points. From this, the expectation of some polynomial combinations of random variables normally distributed is computed. This is related to quadrature formulas and has strong links with designs of experiments. This is joint work with G. Pistone.

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MS26
On the Geometry of Discrete Exponential Families with Application to Exponential Random Graph Models

There has been an explosion of interest in statistical models for analyzing network data, and considerable interest in the class of exponential random graph (ERG) models. In this talk I will relate the properties of ERG models to the properties of the broader class of discrete exponential families. I will describe a general geometric result about discrete exponential families with polyhedral support. Specifically, I will show how the statistical properties of these families can be well captured by the normal fan of the convex support. I will discuss the relevance of such results to maximum likelihood estimation and apply them to the analysis of ERG models. By means of a detailed example, I will provide some characterization and a partial explanation of certain pathological features of ERG models known as degeneracy. Joint work with S.E. Fienberg and Y. Zhou.

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MS26
Introduction to Algebraic Statistics

I will provide an introduction to one of the main principles of algebraic statistics– that statistical models are semialgebraic sets– and illustrate this idea with examples.

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MS27
Improved Accuracy and Efficiency in Leray-alpha Computations

In this talk I will discuss how some simple, yet fundamentally important changes can be made to numerical algorithms for the Leray-alpha model, which lead to significant improvements in accuracy and efficiency.

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MS27
Uncertainty Quantification for a Two Domain Natural Convection Problem

Numerical algorithms are studied for a Boussinesq model of natural heat convection in two domains, motivated by the dynamic core of climate models. One (monolithic) algorithm is coupled across the fluid-fluid interface. Another is decoupled for parallel implementation using a partitioned time stepping approach which retains unconditional stability, a property not enjoyed by climate codes. Reliability of computations is critical in climate applications. Here, stochastic noise is introduced into two nonlinear coupling terms that play an important role in stability, by modeling them with random variables. Uncertainty quantification is performed for each numerical model via the stochastic collocation method. Comparison is drawn in predicting average surface temperature with a "one-way" coupled algorithm, based on a common climate modeling assumption. Uncertainty in average surface temperature is smallest using the monolithic algorithm and largest using the one-way coupled algorithm.

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MS27

Unconditional Convergence of Extrapolated Crank-Nicolson, Finite Element Method for the Navier-Stokes Equations

Error estimates for the Crank-Nicolson in time, finite element in space (CN-FE) discretization of the Navier-Stokes equations require a discrete version of the Gronwall inequality, which leads to a time-step restriction. Previous convergence analyses of CN-FE with linear extrapolation rely on a similar time-step restriction as the full CN-FE. We show that CN-FE with linear extrapolation is unconditionally convergent in the energy norm. We also show optimal convergence of CN-FE with extrapolation in a discrete $L^\infty(H^1)$-norm and convergence of the corresponding discrete time derivative in a discrete $L^2(L^2)$-norm.

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MS27

Continuum-microscopic Interaction Computation of Viscoelastic Turbulent Flow

A continuum-microscopic approach is presented for computing dilute polymer flow at high Reynolds number. The finitely extensible nonlinear elastic (FENE) model is adopted to describe the polymer. The continuum conservation equations require a closure based upon the microscopic configuration state of the polymer. A fast computational method to obtain the closure is presented based upon a multiphysics PARAREAL approach that simultaneously solves stochastic differential equations for the polymer state and a Fokker-Planck equation for the probability distribution function of the states. The PARAREAL algorithm is implemented on graphical processing units. The microscopic configuration of the polymer is investigated at maximum drag reduction conditions.

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MS28

Numerical Methods for a Problem arising in 3D Breast Image Reconstruction

Digital tomosynthesis imaging, the process of reconstructing a 3D object from a few 2D projection images, is a viable alternative to standard mammography in breast cancer imaging. However, current algorithms for image reconstruction do not incorporate the polyenergetic nature of the x-ray beam entering the object, resulting in reconstruction inaccuracies. In this talk, we discuss a novel mathematical model based on a polyenergetic x-ray spectrum and develop statistically based iterative optimization methods for image reconstruction.

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MS28

Modeling Combustion Reactions with Step-function Kinetics

Here we develop reaction-diffusion models for self-propagating reactions where the reaction rates are reduced to have a step-function dependence on temperature. This approach is first studied in the case of a single reaction in both adiabatic and non-adiabatic environments. Of particular interest, however, are systems of two reactions which are thermodynamically coupled. This includes parallel, competing and sequential reactions with both analytical and numerical studies.

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MS28

Non-linear Wave Interactions in Rotating Stratified Fluid Flow

By utilizing the asymptotic renormalization theory of Wirosoetisno et. al. (2002), we propose a dynamical explanation of the origin, nature, and energetics of the spontaneously generated inertia gravity waves which appear in the trough of the baroclinic mode in the rotating annular experiment of Williams et. al. (1995). We compute the $O(\epsilon)$ Wirosoetisno et. al. correction term to the underlying quasi-geostrophic dynamics and compare our results with the location, amplitude, and morphology of the IGWs observed in the lab. We also present energy results which o?er a strong indication that in a real ?uid, spontaneously emitted IGWs are an extremely efficient way to transfer geostrophic energy to ageostrophic energy, ultimately to be dissipated by viscosity

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MS28

The Mechanical Stability of Growing Arteries

In many cylindrical structures in biology, residual stress fields are created through differential growth. The possible role of axial residual stress in regulating stress in arteries and preventing buckling instabilities is investigated. It is shown that axial residual stress lowers the critical internal pressure leading to buckling and that a reduction of axial loading may lead to a buckling instability which may eventually lead to arterial tortuosity.

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MS29

An Implicit Asymptotic Preserving Maxwell Solver

We present an extension of the Boundary Integral Treecode (BIT), a grid free electrostatic O(N log N) field solver, to an implicit electromagnetic field solver. The new method computes a magnetic field that is by construction divergence free in the computational domain. The implicit Maxwell solver is Asymptotic Preserving, recovering the Darwin limit of Maxwell's equations in the long time limit. The method is used to simulate the wave equation for a range of geometries.

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MS29

Quadrature-based Moment Methods for Gas-particle Flows

Gas-particle flows can be modeled by a kinetic equation (KE) for the particle velocity distribution function. The KE contains terms for acceleration due to fluid drag and gravity, transport due to the particle velocity, and inelastic particle-particle collisions. The KE is coupled to the continuity and momentum equations for the gas phase through the particle volume fraction and fluid drag, respectively. In most practical gas-particle flows, the particle Knudsen and Mach numbers are far from the equilibrium limit so that hydrodynamic descriptions of the KE are invalid. In this talk we describe how quadrature-based moment methods can be used to capture non-equilibrium solutions to the KE. Examples for gas-particle riser flows ranging from very dilute to moderately dense particle hold up will be used to illustrate the quadrature-based numerical methods.

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MS29

A High-order WENO Method for the Vlasov-Maxwell System

In this talk, we propose a high-order Vlasov-Maxwell solver based on high-order Runge-Kutta scheme in time and high-order WENO (weighted essentially nonoscillatory) reconstruction in space. The spatial WENO reconstruction developed for this method is conservative and Lax- Friedrichs flux is employed. While the third, fifth, seventh and ninth order reconstructions are presented in this talk, the scheme can be extended to arbitrarily high order. WENO reconstruction is able to achieve high-order accuracy in smooth parts of the solution while being able to capture sharp interfaces without introducing oscillations. The quality of the proposed method is demonstrated by applying the approach to classical plasma problems, such as Weibel's instability. Our numerical results suggest the use of high-order schemes in both time and space is advantageous when considering the Vlasov-Maxwell system.

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MS29

A Hybrid Method for Particle Transport Based on a Collided/ Uncollided Split

We present methods for solving particle transport problems by splitting the phase space density into particles that have collided during a time step and particles that have not collided in the step. Using this paradigm we can exploit benefits of particular methods: moment based methods behave well for particles that have undergone many collisions whereas other methods such as Monte Carlo and integral methods are inefficient in the absence of collisions. We analyze our splitting technique and apply it to several problems of interest in linear transport and radiative transfer.

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MS30

A Least Squares Interpolation Method for Parameterized Systems of Equations

Exhaustive parameter studies for engineering models are typically infeasible, particularly for high dimensional parameter spaces; cheap and accurate surrogate models are necessary. We propose a reduced basis method for approximating the model output given a set of snapshots. The method requires only the residual of the model and poses a least squares problem to compute the coefficients of the approximation. We derive the method in the linear case and extend its application to nonlinear problems

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MS30

A Geometric Interpretation of Stochastic Processes

The time-dependent stochastic harmonic oscillator can geometrically be described as the Lie-derivative of a 1-form on a cylinder, $[a, b] \times S^1$

$$\mathcal{L}_X \alpha^{(1)} = 0 \ ,$$

where $\alpha^{(1)}$ is the 1-form which describes the probability distribution and X is the vector field on the cylinder. This equations means that $\alpha^{(1)}$ does not change along the flow generated by X. In this talk a discrete polynomial representation of differential forms will be given which possesses the invariance under general transformations. As a consequence, integrals are preserved.

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MS30

Proper Generalized Decomposition and Separated Representations for Uncertainty Propagation

A family of model reduction methods, called Proper Generalized Decompositions methods, has been recently proposed for the propagation of parametric uncertainties in very high dimensional stochastic models. It is based on the a priori construction of separated representations of the solution of stochastic partial differential equations. They can be seen as generalizations of Karhunen-Loève decompositions. Here, we review basic definitions of decompositions and propose new definitions in order to improve convergence properties of separated representations.

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MS30

Practical Rare Event Simulation in High Dimensions

I will discuss an importance sampling method for certain rare event problems involving small noise diffusions. Standard Monte Carlo schemes for these problems behave exponentially poorly in the small noise limit. Previous work in rare event simulation has focused on developing, in specific situations, estimators with optimal exponential variance decay rates. I will introduce an estimator related to a deterministic control problem that not only has an optimal variance decay rate under certain conditions, but that can even have vanishingly small statistical relative error in the small noise limit. The method can be seen as the limit of a well known zero variance importance sampling scheme for diffusions which requires the solution of a second order partial differential equation. I will also report on progress toward applying the algorithm within the design of magnetic memory devices.

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MS31

Self-correcting Estimates from the Differential Equations Method

In this talk we discuss applications of the differential equations method for random graph processes in which the bounds on variation around the expected trajectory decrease as the process evolves. These methods are illustrated in the context of the random greedy algorithm for constructing a large partial Steiner-Triple-System. This stochastic graph process is defined as follows: We begin with a complete graph on n vertices and proceed to remove the edges of triangles one at a time, where each triangle removed is chosen uniformly at random from the collection of all remaining triangles. The process terminates when it arrives at a triangle-free graph. We show that with high probability the number of edges in the final graph is at most $O(n^{7/4} \log^{5/4} n)$.

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MS31

A Probabilistic Technique for Finding Almost Periods in Additive Combinatorics

We (E. Croot and Olof Sisask) introduce a new probabilistic technique for finding 'almost periods' of convolutions of subsets of finite groups. This allows us to give: a new probabilistic proof of Roth's theorem; a new way to approach the 2D corners problem; a new result on the existence of long arithmetic progressions in sumsets A+B; a translation-invariance result for "discontinuous sets' (sets A whose convolution function A*A is somewhat discontinuous); and several non-abelian analogues of classical theorems. In many cases, the proofs we give are the shortest known, and in some cases, like the case of long APs in A+B, we obtain the strongest bounds to date.

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MS31

Maximal Independent Sets in Graphs with No Quadrilaterals

There has recently been substantial attention on studying the problem of studying the size of a maximal independent set in a d-regular graph of girth g. The most precise results for large girth and fixed d are recent, due to Gamarnik and Goldberg, following from an analysis of a natural randomized greedy algorithm, and generalizing earlier results of Lauer and Wormald. In this talk I will present a new result stating that every d-regular n-vertex graph containing no cycles of length four contains a maximal independent set I such that

$$\frac{|I|}{n} = \frac{\log d + O(1)}{d}$$

and this is best possible in light of random regular graphs containing no cycles of length four, and in view of unions of complete bipartite graphs with d vertices in each part. In particular, this shows that it is the lack of cycles of length four in a random d-regular graph which gives maximal independent sets of this size. The degree ratio of a graph G is defined to be the maximum degree divided by the minimum degree. We show that there are n-vertex graphs with degree ratio $c > 1$ and maximum degree d such that every maximal independent set has size at least roughly $n/2d^{2/(c-1)}$, which shows that the condition of regularity is necessary in the above-mentioned result. We conjecture that such graphs should have maximal independent sets of size at most $n/2d^{1/c}$ up to logarithmic factors in d for each $c > 1$. Some possible applications of the result will be mentioned.

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MS31

Optimal Inverse Littlewood-Offord Theorems

Let $\eta_i, i = 1, \ldots, n$ be iid Bernoulli random variables, taking values ± 1 with probability $\frac{1}{2}$. Given a multiset V of n integers $v_1, \ldots, v_n$, we define the *concentration probability* as

$$\rho(V) := \sup_x Pr(v_1\eta_1 + \ldots v_n\eta_n = x).$$

A classical result of Littlewood-Offord and Erdős from the 1940s asserts that if the v_i are non-zero, then $\rho(V)$ is $O(n^{-1/2})$. Since then, many researchers obtained improved bounds by assuming various extra restrictions on V. About 5 years ago, motivated by problems concerning random matrices, Tao and Vu introduced the Inverse Littlewood-Offord problem. In the inverse problem, one would like to give a characterization of the set V, given that $\rho(V)$ is relatively large. In this talk, I describe a new method to attack the inverse problem. As an application, we strengthen a previous resultof Tao and Vu, obtaining an optimal characterization for V. This characterization immediately implies several classical theorems, such as those of Sárközy-Szemerédi and Halász. As another application, we obtain an asymptotic, stable version of a famous theorem of Stanley that shows that under the assumption that the v_i are different, $\rho(V)$ attains its maximum value when V is a symmetric arithmetic progression. All results extend to the general case when V is a subset of an abelian torsion-free group and η_i are independent variables satisfying some weak conditions. The method also works well in the continuous setting, and gives a simple proof for the β-net theorem of Tao and Vu,

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MS32

RBF Solution of Lid-Driven Cavity Problem using the Stream Function Formulation.

An RBF meshless formulation of the lid-driven cavity problem is presented. It uses the streamfunction-vorticity formulation so that the problem reduces to the solution of a nonlinear biharmonic equation describing the stream function. For the Stokes problem ($Re = 0$), the accuracy deteriorates in the neighborhood of the singularities in the two upper corners. Enlarging the space spanned by the RBF basis functions with additional functions that capture the singular behavior of the solution restores the spectral convergence of the RBF method.

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MS32

Approximation of Linear PDEs by Gaussian Processes via Matérn Functions

Given discrete data $X_1 = \{x_i\}_{i=1}^N \subset \Omega$, $X_2 = \{x_{N+j}\}_{j=1}^M \subset \partial\Omega$ and $Y = \{f_k(x_i), g_l(x_{N+j})\}_{i,j,k,l=1}^{N,M,n,m}$ generated from a linear partial differential equations model

$$\begin{cases} L_1u(x) = f_1(x), \cdots, L_nu(x) = f_n(x), & x \in \Omega, \\ B_1u(x) = g_1(x), \cdots, B_mu(x) = g_m(x), & x \in \partial\Omega, \end{cases}$$

where L_k are linear differential operators, B_l are linear boundary operators and Ω is a bounded domain in $\mathcal{R}^\lceil$. A Gaussian process (Gaussian field) is firstly constructed on a reproducing-kernel Hilbert space corresponding to a Matérn function. Combining this with a Bayesian approach, we are able to obtain confidence interval for $u(x)$ (instead of an explicit approximating solution) through a covariance matrix for the above differential operators and boundary operators on the data.

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MS32

RBF Interpolation using Gaussians with Domain Decomposition on GPUs

We have developed a parallel algorithm for radial basis function (RBF) interpolation with Gaussians that uses a GMRES iterative solver with a restricted additive Schwarz method (RASM) as a preconditioner and a fast matrix-vector algorithm. The fast decay of the Gaussian basis function allows rapid convergence of the iterative solver, while retaining the interpolation accuracy. The preconditioning and matrix-vector product have been ported to CUDA to accelerate the most computationally intensive parts of the algorithm.

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MS33

Nonlinear Model Reduction Using Petrov-Galerkin

Projection and Data Reconstruction

A computational method for constructing a stable nonlinear reduced-order model and analyzing it as fast as possible is presented. This method operates on a semidiscretized partial differential equation, relies on a time-variant Petrov-Galerkin projection for performing model reduction, and on a reconstruction of gappy data for approximating the reduced system in order to accelerate its analysis. Its performance is highlighted for sample problems in nonlinear structural dynamics and computational fluid dynamics

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MS33

Interpolation for Adaptation of Parameterized Reduced-Order Models

Differential geometry-based interpolation methods are presented for adapting parameterized reduced-order models to new configurations. Two different approaches are discussed. The first one is based on the interpolation of the underlying reduced-order bases, and the second one on the interpolation of the reduced-order models themselves. It is shown that the first approach privileges robustness and stability at the expense of CPU time, whereas the second approach delivers real-time performance at the expense of generality and robustness.

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MS33

A Projection-based Moment-matching Interpolation for Large-scale Frequency Response Problems

Frequency response problems appear in many computational engineering applications. Our attention is focused on evaluating functions $\mathbf{H}(\sigma) = (\mathbf{K} + \mathbf{i}\sigma\mathbf{D} - \sigma^{\mathbf{2}}\mathbf{M})^{-\mathbf{1}}\mathbf{f}$ on an interval $[\sigma_l, \sigma_r]$. The matrices $\mathbf{K}$, $\mathbf{D}$, and $\mathbf{M}$ are very large and they may have complex entries. We will present a method that exploits values of $\mathbf{H}$ and its derivatives at multiple frequencies to construct a reduced-order model for $\mathbf{H}$, with a rational Krylov algorithm. The computations of values and derivatives of $\mathbf{H}$ at multiple frequencies will use a domain-decomposition based iterative solver for large-scale indefinite systems. Numerical experiments from structural dynamics and fluid-structure interaction problems will illustrate the method.

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MS33

Nonlinear Model Reduction for Porous Media Flow

A Discrete Empirical Interpolation Method (DEIM) is applied in conjunction with Proper Orthogonal Decomposition (POD) to construct a nonlinear reduced-order model of finite difference discretized system used in the simulation of nonlinear miscible viscous fingering in a 2-D porous medium. POD is first applied to extract a low-dimensional basis that optimally captures the dominant characteristics of the system trajectory. This basis is then used in a Galerkin projection scheme to construct a reduced-order system. DEIM is then applied to greatly improve the efficiency in computing the projected nonlinear terms in the POD reduced system. DEIM achieves a complexity reduction of the nonlinearities which is proportional to the number of reduced variables while POD retains a complexity proportional to the original number of variables. Numerical results demonstrate that the dynamics of the viscous fingering in the full-order system of dimension 15000 can be captured accurately by the POD-DEIM reduced system of dimension 40 with the computational time reduced by factor of 1000.

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MS34

Correctors and Field Fluctations for the $p_\epsilon(x)$-Laplacian With Rough Exponents

We provide a corrector theory for the strong approximation of fields inside composites made from two materials with different power law behavior. The correctors are used to develop bounds on the local singularity strength for gradient fields inside micro-structured media. The bounds are multi-scale in nature and can be used to measure the amplification of applied macroscopic fields by the microstructure.

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MS34

Simultaneous Seismic Imaging and Inversion Using an Inverse Scattering Algorithm for One Dimensional Media

We present the theoretical development and numerical tests for an acoustic inverse scattering algorithm for simultaneous geophysical imaging and amplitude correction directly from measured data. No knowledge about the medium under investigation is assumed. We model several one-dimensional earth configurations and show how the algorithm can find the precise location and a good estimate of the layers' parameters. Our tests will include different number of layers, high/low contrasts, velocity inversions and noisy data.

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MS34

A Split Sparse/Dense Matrix-vector Multiplication Routine

A new approach for performing sparse matvecs consists of two stages: (i) reordering the original general sparse matrix A, and (ii) tearing it into two parts – a dense banded matrix B and a sparse matrix E of much lower rank. The multiplication of B by a block of vectors is accomplished via dense BLAS level-3. Comparisons are made against Intel's MKL matvec routine, mkl_csrmm, and an extension using multi-level splitting will be discussed.

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MS34

Understanding the Impact of Low Permeability Media on Groundwater Remediation

In groundwater remediation, contaminants trapped in low permeability soil after clean-up can cause re-contamination in the same area after a long period of time. This study focuses on analyzing and improving existing transport models to understand the contaminant behavior in terms of the rate and extent of release from its storage at the HPM/LPM interface. Current approaches include a sensitivity analysis of MT3D model, constructing a numerical simulator using dual-resistance model, and lab cell experiments.

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MS34

Option Pricing Using Monte Carlo Methods

One main problem in mathematical finance is calculating the fair price of derivatives. The fair price of these derivatives can be complicated to obtain analytically. Monte Carlo simulation offers a way to compute the fair price, relying on the approximation of an expected value by the average of the simulated values. We created a random number generator and used it in the Monte Carlo simulations to compute the fair price of a European Call Option.

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MS34

A Novel Pseudospectral Method for Solving a Nonlinear Volterra Partial Integro-differential Equation on a Polar Geometry

In this talk we study a nonlinear Volterra partial integrodifferential equation used to model swelling porous materials where the problem domain is a unit disk. We show well-posedness is established under a given set of assumptions and introduce a novel approach to constructing pseudospectral differentiation matrices in a polar geometry for computing the spatial derivatives. An exponential time-differencing scheme proposed by Cox and Matthews and stabilized by Kassam and Trefethen is employed for the time-stepping.

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MS35

Tensor Decomposition and Application in Signal and Image Processing

We describe a module of n-by-n matrices upon which every linear transformation can be represented by tensor-matrix multiplication by a third-order tensor. An inner product is defined upon this space, which leads to natural extensions of many familiar linear algebra concepts including length and orthogonality of matrices and symmetry of tensors. Using these tools, we investigate applications in the areas of image reconstruction and pose estimation.

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MS35

Tensor-SVD with Applications in Image Processing

We define a new type of multiplication between two tensors that allows for the representation of tensors as products of tensors that is reminiscent of matrix factorizations. In particular, a tensor-SVD is introduced which gives a representation of tensors as the sum of outer-products of matrices. This alternate representation of tensors shows promise with respect to the tensor approximation problem in the context of image processing. We test our approach on an image deblurring application.

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MS35
Iterative Methods for Multilinear Systems

We have shown a tensor group endowed with the Einstein (contracted) product is isomorphic to the general linear group of degree n. In consequence, higher order tensor inversion is possible for even order. Although odd order tensors are not invertible under the Einstein product, their inversions are still possible through pseudo-inversion techniques. With the notion of tensor inversion, multilinear systems are solvable. Numerically we solve multilinear systems arising from partial differential equations and quantum mechanics. Iterative methods for tensors are the main computational techniques. We demonstrate the efficacy of these iterative methods through some motivating examples.

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MS35
Tensors as Module Homomorphisms over Group Rings

Abstract not available at time of publication.

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MS36
On Multirate SSP Methods for Hyperbolic PDEs

We discuss a set of explicit multirate time discretization methods for hyperbolic conservation laws based on multistep and Runge-Kutta methods. Multirate methods allow different time steps to be used in different parts of the spatial domain while preserving the consistency and conservation properties of the "classical" methods. Linear and nonlinear stability are guaranteed only under local CFL conditions. The necessity to take small global time steps restricted by the largest CFL number is thus avoided. The theoretical results are illustrated on advection and Burgers equations.

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MS36
The History of SSP Methods

Abstract not available at time of publication.

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MS36
On the Sharp SSP Timestep for Runge-Kutta Discretizations of IVPs

The product of the absolute monotonicity radius of the Runge-Kutta (RK) method and the strong stability preserving (SSP) timestep of the explicit Euler method is often used as a timestep limit that guarantees strong stability preservation of the RK method. In this talk we relax this limit in two ways. First, for certain subsets of the initial vector we prove that in the above limit a much larger factor than absolute monotonicity rules the SSP property. Second, for some classical RK methods we prove SSP property also in the case when the explicit Euler method is not SSP for any positive timestep. Finally, we demonstrate our results by computational experiments.

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MS36
Multi-step Multi-stage SSP Runge–Kutta Methods

High-order strong stability preserving (SSP) time integrators of are often desirable in the numerical solution of hyperbolic PDEs. Multistep Runge–Kutta methods generalize both linear multistep methods and multistage Runge–Kutta methods. We present some recent results on SSP multistep Runge–Kutta methods, including numerically optimal methods, both implicit and explicit. The methods are tested with numerical experiments.

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MS37

Hydrodynamics Coupled with Bed Morphology for Modeling Sediment Scour and Deposition

Abstract unavailable at time of publication.

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MS37

Adaptive Strategies in the Multilevel Multiscale Mimetic (M^3) Method for Two-phase Flows in Porous Media

The Multilevel Multiscale Mimetic (M^3) method was developed to simulate accurately two-phase flows in highly heterogeneous media with long correlation lengths. A multilevel approximation strategy is used to build a hierarchy of models that are locally conservative at each level. The mimetic finite difference method is used to handle arbitrary meshes and tensor permeability fields. We describe adaptive strategies that reduce further the cost of the M^3 method and illustrate them with numerical simulations of well-driven flows.

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MS37

Stochastic Multiscale Modeling of Coupled Surface-subsurface Flow and Contaminant Transport

We discuss a multiscale stochastic framework for uncertainty quantification in modeling flow and transport in surface-subsurface hydrological systems. The governing flow equations are the Stokes-Darcy system with Beavers-Joseph-Saffman interface conditions. The permeability in the Darcy region is stochastic and it is represented with a Karhunen-Loève (KL) expansion. The porous media can be statistically non-stationary, which is modeled by different KL expansions in different regions. Statistical moments of the solution are computed via sparse grid stochastic collocation. The spatial domain is decomposed into a series of small subdomains (coarse grid) of either Stokes or Darcy type. The flow solution is resolved locally (on each coarse element) on a fine grid, allowing for non-matching grids across subdomain interfaces. Coarse scale mortar finite elements are introduced on the interfaces to approximate the normal stress and impose weakly continuity of flux. The transport equation is discretized via a local discontinuous Galerkin method. Computational experiments are presented.

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MS37

Stochastic Collocation Data Assimilation

In this work, a stochastic data assimilation approach is presented for estimating model parameters such as permeability and porosity from direct and indirect measurements. This approach combines the advantages of the ensemble Kalman filter (EnKF) for dynamic data assimilation and the polynomial chaos expansion (PCE) for efficient uncertainty quantification. In the latter, the model parameters are represented by the Karhunen-Loeve expansions and the model responses such as pressure and saturation are expressed by the PCE. The coefficients of PCE are solved with a collocation technique. The approach is non-intrusive in that such realizations are solved forward in time via existing deterministic solver independently. The needed entries of the state covariance matrix are approximated with the PCE coefficients. It is shown that the approach is computationally efficient and provides satisfactory estimations of the model parameters with dynamic measurements.

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MS38

Adaptive Rational Krylov Subspaces for Time-invariant Dynamical Systems

The rational Krylov space is recognized as a powerful tool within Model Order Reduction techniques for linear dynamical systems. However, its success has been hindered by the lack of procedures, which would generate the sequence of shifts used to build the space with good approximation properties. We start with a-priori and adaptive approaches generating such shifts for the first order problems. Then a-priori approach is generalized to structure preserving algorithms for high order systems.

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MS38

Robust Low-order Models for Flow Control

The main issue discussed will be how to build a low-order model that is robust to parameter variation. To do that an optimal sampling strategy of the parameter space based on the full model residuals is proposed. In addition to that, the reduced model is calibrated using Tikhonov regularization. This system identification approach can accurately describe unsteady phenomena encountered in flow control.

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MS38

Model Reduction Algorithm for Robust Control of Linear PDE Systems

We consider the computation of a robust control law for large-scale finite dimensional linear systems and a class of linear distributed parameter systems. The controller is robust with respect to left coprime factor perturbations of the nominal system. We present a convergent algorithm based on balanced proper orthogonal decomposition to compute the nonstandard features of this robust control law. Numerical results are presented for a convection diffusion partial differential equation.

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MS38

Model Order Reduction for Steady Aerodynamic Applications

An approach combining proper orthogonal decomposition (POD) with linear regression, which is called gappy POD, is used to obtain complete flow solutions in steady aerodynamic applications from knowledge of a (suitable) POD basis and the solution at very few points. In practice the partial or gappy data can easily be obtained by experimentally measuring the flow variables. Therefore this method is effective in combining experimental with computational data.

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MS39

A Geometric Approach to Partition Functions

Computing partition functions to get normalizing constants or marginals is an ubiquitous, yet generally intractable, task in statistical modelling. Many tricks and workarounds have been developed to make such computations feasible. I discuss how some of these strategies can be understood, and new ones manufactured, using tensor geometry.

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MS39

Combinatorial Commutative Algebra in Action: Markov Moves from Classical Algebraic Constructions

Markov bases, as a fundamental object of study in algebraic statistics, can often be difficult to construct and compute. It is often the case that a sub-basis may be sufficient for the problem at hand; however, theoretically, one would like to really understand the variety of the model, its algebraic and geometric properties. In this talk I will describe challenges in Markov bases constructions, posed by the poorly understood geometry of the models, illustrated on an example.

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MS39

Algebraic Statistics Framework for Causal Inference and Data Privacy with Discrete Data

We present an algebraic computational framework that handles special cases of latent class analyses. Specifically, we consider discrete data problems with unobserved variables such that arbitrary linear constraints are imposed on the possible realizations of the complete data, and thus on the possible states of the joint distribution of all the variables (observed and unobserved) in the analysis. The constraints are imposed either by the modeling assumptions, the structure of the latent variables or for consistency reasons. We illustrate our methods by applying them to two important related problems. The first problem pertains to the assessment of disclosure risk of releasing potentially sensitive information from a latent class analysis in the form of class membership probabilities and probability distribution of covariates conditional on the classes. The second problem pertains to estimation of average causal effect in presence of unobserved confounders , under the Neyman-Rubin framework of potential outcomes. The code is implemented in R, but interfaces with 4ti2.

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MS39

Betti Numbers of Experimental Designs

For polynomial regression models in the context of factorial experimental design there have been both formal and informal way of representing estimable effects and interactions. We generalize this to a larger study of the combinatorial structure of models derived by the algebraic method, that is using ideals-of-points theory. It turns out, by exploiting known results on monomial ideals, that the complexity of models can be measured by the size of the Betti numbers of the Stanley-Reisner complex. It transpires that the most complex models are available for designs which are generic in the sense of 'corner cut' theory. An complete enumeration for Plackett-Burman designs gives 19 equivalence classes of complex.

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MS40

Dual-mixed Finite Element Methods for the Navier-Stokes Equations

In many applications within mechanical, materials, and biomedical engineering, it is important to accurately predict fluid stresses. However, most existing numerical schemes for fluids are formulated with velocity as the primary unknown of interest. In this talk, a dual-mixed finite element method for the Navier-Stokes equations, in which the stress is a primary unknown of interest, is derived and analyzed. The method employs symmetric tensor finite elements for stress and is well-suited for non-Newtonian fluids.

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MS40

Local Boundary Condition based Spectral Collocation Methods for 2D and 3D Naiver-Stokes Equations

We present a simple approach to accurately computing local boundary conditions in spectral collocation schemes for the Navier-Stokes equations in 2D and 3D. Access to these local boundary values makes possible the decoupling of the computation of the primary flow variables, resulting in highly efficient schemes. In 2D the local vorticity boundary values are employed in the vorticity-stream function formulation, while in 3D local values of a Neumann boundary condition for the pressure in the velocity-pressure formulation are used. In both cases these boundary conditions are approximated by differentiating a local Lagrange interpolant at the boundary. The straightforward extension of the approach to the Boussinesq system is also discussed. The resulting schemes are well suited for the simulation of moderate to high Reynolds and Rayleigh number flows. Accuracy checks, simulations of the lid-driven cavity flow, of a differentially heated cavity flow, and of a Rayleigh-Bernard convection problem for Rayleigh number up to 10^{10} are presented to demonstrate that the schemes are capable of producing accurate results at a reasonable computational cost.

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MS40

Numerical Approximation for Generalized-Newtonian Flows with Flow Rate Boundary Conditions

We consider a generalized-Newtonian fluid with defective boundary conditions where only flow rate are prescribed on a part of boundary. The defect boundary condition problem is formulated as an minimization problem in which a Neumann or Dirichlet boundary control is used for the flow rate matching. We will discuss the derivation of an optimality system based on the first necessary condition and examine the corresponding adjoint problem. Computational algorithms and numerical results will be also presented.

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MS40

Optimal Control of Flow Past a Rectangle

We address optimal control of the frequency and amplitude of two-dimensional vortex-shedding behind a rectangular obstacle. Control is effected by small periodic oscillation of the rigid obstacle. Numerical results are presented.

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MS41

Using Sequence Coverage Statistics to Determine Protein Binding Sites in a Genome

Inspired by the notion of persistence in topological data analysis, we introduce a tree depicting sequence coverage via fragment placement on a genome. We then describe statistically the trees that correspond to random fragment placement and use this theory to determine the binding sites for a given protein in a genome. Our method for calling statistically signi?cant protein binding sites reduces to the study of certain tree-based statistics derived from the data.

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MS41

Lower and Upper Bounds on the Probability Distributions of the Wasted Spaces of a Processor-Sharing Storage Allocation Model

We consider a storage allocation model with m primary holding spaces, infinitely many secondary ones, and one processor servicing customers. We define the traffic intensity ρ to be λ/μ where λ is the customer arrival rate and μ is the service rate of the processor. We study the lower and upper bounds on the probability distributions of the wasted spaces and the largest index of the occupied spaces for fixed rho, $0 < \rho < 1$, and $\rho = 1 - \epsilon$ (heavy traffic case).

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MS41

Mechanisms of Simple Perceptual Decision-making Processes

Perceptual decision-making, an omnipresent component of everyday life, plays a pivotal role in cognitive tasks. In this presentation, I will talk about mechanisms underlying simple two-option perceptual decision-making processes by studying a biological-realistic reduced two-variable model and phenomenological drift-diffusion models.

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MS41

Oscillations in NFkB Signaling Pathway

Upon stimulation, oscillations of NF-kB localization are observed at both single cell and population levels. A recent work reported that different frequencies of the oscillations leads to different gene expression. Many authors point out that NF-kB may interact with other pathways. However, the existence and mechanism of those potential interactions are not clear. In this talk, we study this issue by considering the pathway subjected to two types of putative signals: sinusoid and pulsatile signals.

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MS42

Numerical Methods for Solving Polynomial Systems

The term numerical algebraic geometry describes a variety of numerical methods for finding and manipulating the solution sets of polynomial systems. There are numerous applications throughout the sciences and engineering as well as many within mathematics. This talk will serve as a brief introduction to some of these methods and applications, including some open problems. This talk (in fact, the entire minisymposium) is intended to support the plenary lecture of Charles Wampler.

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MS42

Regeneration and Numerical Algebraic Geometry

Large-scale polynomial systems that often arise in kinematics and other engineering applications typically have fewer solutions than their total degree root count. Regeneration can solve such large-scale polynomial systems by algorithmically revealing the underlying structure of the polynomial system during the equation-by-equation solving process. After describing regeneration, we will apply it to polynomial systems arising in kinematics and other engineering applications.

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MS42

Basic Algebraic Geometry of Acoustic Arrays

This talk is on the basic algebraic geometry of acoustic arrays. Given an array of microphones and a point P there is a set of time delays that, when applied to the signals collected by the microphones, lead to a focusing of the microphones towards P. The locus of such coherent time delays determine an algebraic variety. We will discuss this variety, an associated moduli space and will discuss themes in common with kinematic varieties.

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MS42

Numerical Matrix Computation in Algebraic Geometry

Numerical polynomial algebra and numerical algebraic geometry become fast growing fields of studies where tremendous progress has been achieved and new challenges emerge (e.g. handling ill-posedness). On the other hand, numerical polynomial algebra is a natural extension and an application area of numerical linear algebra, as matrix computation plays an indispensible role. This talk introduces the matrix computation strategies in numerical polynomial algebra and numerical algebraic geometry using several case studies along with computing results.

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MS43

Hybrid Monte Carlo Methods for Kinetic Equations

Probabilistic techniques such as DSMC (Direct Simulation Monte Carlo) are extensively used in real simulations of the Boltzmann equation for their great flexibility, ability in treating different collision terms and low computational cost compared to any type of deterministic scheme. On the other hand, solutions are affected by large fluctuations and, in non stationary situations, the impossibility of averaging quantities leads to, or low accurate solutions, or high costly simulations. Moreover, close to thermodynamical equilibrium, the cost of Monte Carlo methods increases. In this talk, emphasis will be addressed to a recent developed new family of Hybrid Monte Carlo methods which permits to treat both accurately and fast transitional regimes and multiscale problems. The key aspects, on which methods rely, are the choice of a suitable hybrid representation of the solution and a merging of Monte Carlo methods in non-equilibrium regimes with deterministic methods in equilibrium ones.

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MS43

An Asymptotic Preserving Scheme for Non-classical Particle Transport

We present a numerical scheme to solve the nonclassical particle transport model suggested by Larsen [Larsen, A generalized Boltzmann equation for non-classical particle transport, ANS M&C 2007]. This model has applications in radiative transfer through clouds and novel nuclear reactor types. While basically any scheme for linear transport has a diffusion limit (albeit with the wrong diffusion coefficient), we show here that the discretization of the transport part has to be chosen carefully so that the scheme has a (correct) diffusion limit.

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MS43

Numerical Simulations of Radiative Shock Tube Experiments: Challenges and Approaches

The Center for Radiative Shock Hydrodynamics (CRASH) investigates ways to improve the predictive capability of models for shock waves produced when a laser is used to shock, ionize, and accelerate a beryllium plate into a xenon-filled shock tube. These shocks, when driven above a threshold velocity of about 100 km/s, become strongly radiative and convert most of the incoming energy flux to radiation. What results is a complex, evolving, radiation-hydrodynamic, multiphysics environment. I will discuss the challenges and approaches we use to model this system as a tractable problem in large-scale parallel computing.

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MS43

High-order Discontinuous Galerkin Schemes for 2+2 Vlasov Models on Unstructured Grids

The purpose of this work is to explore mesh-based alternatives to the Particle-In-Cell (PIC) methods that are currently favored in many plasma physics applications. In particular, we present here a technique for solving the Vlasov-Poisson system that is based on operator splitting in time and high-order discontinuous Galerkin discretizations in space. The efficiency of the method is increased by considering semi-Lagrangian approaches for the advection in phase space. The flexibility of the approach is enhanced by allowing the mesh in physical space to be unstructured.

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MS44

Asynchronous Time Integration for Periodic Dynamical Systems with Uncertain Parameters

Application of PC expansions to stochastic dynamical systems exhibiting cyclic oscillations frequently leads to a broadening solution spectrum, and consequently to excessive computational requirements. This talk outlines an asynchronous integration framework that offers to substantially mitigate this problem. The approach is based on a stochastic time rescaling which is implemented so that the spectrum of the rescaled solution remains narrow-banded. Different variants of this approach are illustrated for simple systems having almost surely a stable limit cycle, including a stochastic linear oscillator, and a stiff nonlinear chemical system with uncertain rate parameters.

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MS44

Phase Conditions for Autonomous Oscillators with Random Parameters

We consider autonomous systems of ordinary differential equations (ODEs) or differential algebraic equations (DAEs), which exhibit periodic solutions. Since a continuum of periodic solutions exists, we require a phase condition to isolate a particular solution. We assume uncertainties in some parameters of the autonomous systems. Hence the relevant parameters are replaced by random variables. We apply the technique of the generalized polynomial chaos to resolve the stochastic model. A Galerkin approach yields a larger coupled system of ODEs or DAEs. The phase conditions of the original systems imply additional boundary conditions in the periodic problems of the larger coupled systems. However, the expected value and the variance of the solution depend on the choice of the phase condition. We construct an alternative constraint, which minimizes the variance of the solution. Numerical simulations of a test example are presented.

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MS44

Eigenvalue Analysis of Uncertain ODE Systems

The polynomial chaos expansion provides a means of representing any L^2 random variable as a sum of polynomials that are orthogonal with respect to a chosen measure. Examples include the Hermite polynomials with Gaussian measure on the real line and the Legendre polynomials with uniform measure on an interval. Polynomial chaos can be used to reformulate an uncertain ODE system, using Galerkin projection, as a new, higher-dimensional, deterministic ODE system which describes the evolution of each mode of the polynomial chaos expansion. It is of interest to explore the eigenstructure of the original and reformulated ODE systems, by studying the eigenvalues and eigenvectors of their Jacobians. In this talk, we study the distribution of the eigenvalues of the two Jacobians. We outline in general the location of the eigenvalues of the new system with respect to those of the original system, and examine the effect of expansion order on this distributio

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MS44

Uncertainty Quantification via Codimension One Domain Decomposition and a New Concentration Inequality

We propose a localized variant of McDiarmid's inequality in order to obtain upper bounds on the probability that a system of interest assumes certain values ("fails'). By partitioning the input parameter space appropriately, much sharper bounds than the usual McDiarmid bound are obtained. We prove an error estimate for the method, define a codimension one recursive partitioning scheme and prove its convergence properties, and use a new concentration inequality to give confidence levels when empirical means are used in place of exact ones.

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MS45

Operator Splitting Methods for Maxwell's Equations in Dispersive Media

We consider Maxwell's equations in dispersive media of Debye type. In such relaxing dielectric media, the presence of different wave speeds leads to stiffness in the temporal domain. We present an operator splitting scheme that decouples fast and slow moving processes in the problem to develop separate sub-problems. This alleviates the stringent requirements on the time-step which along with stability conditions requires small spatial steps and hence excessive computations for long-time integration of Maxwell's equations.

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MS45

Overlapping Domain Decomposition Method for the Helmholtz Equation

The model problem addressed in this talk concerns the analysis and computation of a radiated or scattered time-harmonic acoustic solution, where the obstacle is composed of dielectric and metal. A new adaptive radiation condition method, that localizes the artificial interface only around the dielectric object, is described. An appropriate algorithm coupling finite and boundary element methods is solved iteratively using an overlapping domain decomposition method. Numerical results are presented validating the theoretical results.

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MS45

A Numerical Method for Simulating EM Wave Propagation in Dielectrics that Exhibit Fractional Relaxation

The frequency-dependent Havriliak-Negami dielectric permittivity model, $\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{(1+(i\omega\tau)^\alpha)^\beta}$, where $0 < \alpha,\ \beta < 1$, generates the entire class of dielectric models used in numerical simulations of time-domain propagation and scattering of electromagnetic waves. We present a numerical method to incorporate this model in a solver for Maxwell's equations which now contain fractional differential operators. We give a complete stability and error analysis of the method and a validation against the exact solution available in some simple cases.

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MS45

Polynomial Chaos Approach for Approximating Cole-Cole Dispersive Media

Time-domain simulations involving the Cole-Cole model are not straight-forward as the model corresponds to a fractional order ODE. We introduce an alternative approach based on using the first order linear ODE Debye model, but with distributions of relaxation times. We apply generalized Polynomial Chaos, and then discretize the system coupled with Maxwell's equations. We present a stability and dispersion analysis of the overall method and discuss the impact of the variance of relaxation times.

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MS46

Scalable Algorithms for Large-Scale Inverse Wave Propagation

Abstract not available at time of publication.

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MS46

A Regularized Trust Region Model for Ill-conditioned Nonlinear Problems

For ill-conditioned nonlinear problems, we must carefully balance the convergence rate with step-size control for robustness. In particular, the optimization steps must reflect the local nature of the model problem solved in each step. We will show that standard methods such as damped Gauss-Newton, Levenberg-Marquardt, and others tend to make relatively poor steps if the Jacobian (or Hessian) is very ill-conditioned. Based on our analysis, we propose a regularization of the local model problem that leads to much more effective steps. We demonstrate our approach on nonlinear least-squares problems arising in shape-based regularization for diffuse optical tomography.

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MS46

A Numerical Scheme for Monge-Kantorovich Mass Transfer Problem, in the Context of Image Registration

The Monge-Kantorovich mass transfer problem addresses the question of how to move a pile of soil from one location to another with minimal cost. In this work we introduce computationally efficient numerical method for non-rigid image registration based on the optimal mass transport theory. We will consider the formulation of Banemou and Brenier (2000), which requires the solution of a time-dependent PDE constrained optimization, with mass-preserving PDE.

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MS46

Iteratively Regularized BFGS-type Algorithm for an Inverse Problem in Groundwater Hydrology

A novel iteratively regularized BFGS-type algorithm with simultaneous updates of the operator

$$(F'^*(x_n)F'(x_n) + \beta_n G'(x_n - \xi))^{-1}$$

is suggested for solving nonlinear ill-posed operator equations of the first kind $F(x) = f_\delta$, $H_1 \to H_2$, on a pair of Hilbert spaces H_1 and H_2. A convergence theorem is proved. The stability of the process towards noise in the data is analyzed, and a stopping time is chosen so that the method converges as the noise level tends to zero. The proposed scheme is illustrated by a numerical example in which a nonlinear inverse problem of groundwater hydrology is considered.

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MS48

Non-oscillatory Behavior of IMEX Schemes Applied to Hyperbolic Problems

The application of a Method-of-Lines approach to a hyperbolic PDE with stiff source terms gives rise to a system of ODEs containing terms with very different stiffness properties. In such situations, it is convenient to use additive Runge Kutta schemes. Implicit-Explicit Runge-Kutta (IMEX-RK) schemes are particularly useful, because they allow an explicit handling of the convective terms, which can be discretized using the highly developed shock capturing technology, and an implicit treatment of the source terms, necessary for stability reasons. In this talk we are concerned with certain numerical difficulties associated to the use of high order IMEX-RK schemes in a direct discretization of balance laws with stiff source terms. We consider a simple model problem, introduced by LeVeque and Yee in [J. Comput. Phys 86 (1990)], as the basic test case to explore the ability of IMEX-RK schemes to produce and maintain non-oscillatory reaction fronts. In the first part of the talk, we consider first order time discretizations, which are the basic building blocks of higher order IMEX schemes, and we establish a convenient framework to study the non-oscillatory properties of numerically computed reaction fronts. In the second part, we extend the results to higher order IMEX schemes. This is a joint work with R. Donat (Departament de Matemàtica Aplicada, Universitat de València, 46100 Burjassot, Spain, donat@uv.es) and A. Martínez-Gavara (Departamento de Ecuaciones Diferenciales y Análisis Numérico, Universidad de Sevilla, 41012 Sevilla, Spain, gavara@us.es)

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MS48

Optimal Time Integration for Runge-Kutta Discontinuous Galerkin Discretizations

Runge-Kutta discontinuous Galerkin methods typically employ optimal strong stability preserving (SSP) time integrators. Although these integrators are optimized in terms of the SSP coefficient, the practical timestep is governed by linear stability constraints. In order to achieve a larger stable timestep, we develop methods that optimize the minimum of the linear and nonlinear (SSP) timestep constraints. We demonstrate that these methods yield better performance than those obtained by optimizing either one of the SSP coefficient or the linear stability without regard to the other.

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MS48

An Analysis of the Spatial and Temporal Errors of the Local Runge-Kutta Discontinuous Galerkin Method

We analyze the total error of discontinuous Galerkin solutions of one-dimensional scalar hyperbolic problems. We show that the error can be split into two components which can be thought of as temporal and spatial errors. The temporal error is of global character and propagates between mesh cells. The spatial error is local and superconvergent at the roots of the Radau polynomials. Application of these findings to error estimation, error control and adaptivity in space and time will be discussed.

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MS48

SSP Properties of General Linear Methods

Abstract not available at time of publication.

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MS49

Swimming of Waving Cylindrical Rings in a Stokes Fluid

The classical 1952 paper of G.I. Taylor examined the action of a waving cylindrical tail in a Stokes fluid. Motivated by the intriguing function of the dinoflagellate transverse flagellum, we ask the question, what if the cylindrical tail was wrapped into a closed circle? We present numerical studies that address the fundamental fluid dynamics of a waving helical ring in a viscous fluid.

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MS49

Simulation of Permeable Membranes using Regularized Source-doublets

To compute small-scale fluid flows, it is convenient to use regularized versions of known singular solutions. We combine the method of regularized Stokestlet with regularized source-doublets to solve the Stokes equations in the presence of membranes permeable to fluids or to diffusive fluxes. Numerical examples are used to investigate the relationship between the permeability/diffusivity of the membrane and the strength of the source-doublets, and to validate the method.

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MS49

Simulations of Flagellar Motion near a Rigid Surface

We present a computational model for the simulation of Stokes flows generated by forces and torques close to a rigid plane and apply it to study the swimming motion of flagellated organisms near a rigid surface. The model is based on an extension of the method of regularized Stokeslets in which a regularization parameter provides support for forces and torques exerted on the fluid by the organism, and eliminates the singularity of the velocity expressions.

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MS49

The Hydrodynamic Origin of Whale Flukeprints

Whale flukeprints are characteristic smooth oval shaped patches on the surface of the ocean which form behind a whale during cruising or diving. Conjecture for the formation of these flukeprints fall into two categories: surfactant or hydrodynamic based. We present a coherent theory of flukeprint formation which is entirely hydrodynamic in nature. We draw upon our own laboratory experiments as well as many aspects of the literature including mathematical biology, mathematical models, and numerical simulations.

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MS50

A Priori and A Posteriori Analysis of Mixed Finite Element Methods for Nonlinear Elliptic Equations

We study the mixed finite element approximation of nonlinear second-order elliptic problems. Existence and uniqueness of the approximate solution are proved and optimal order *a priori* error estimates in $L^m(\Omega)$ are obtained. Also, reliable and efficient *a posteriori* error estimators measured in the $L^m(\Omega)$-norm are derived. Numerical examples are provided to illustrate the performance of the proposed estimator.

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MS50

Mixed Finite Elements for Deformed Cubes

Mixed finite element methods and the associated cell centered finite volume methods are known to have many advantages for the numerical modeling of flow in porous media. For many problems involving flow in porous media, however engineers prefer to use grids that are deformations of regular grids made up of 3D rectangular solids. Unfortunately the adaptation via the Piola transformation of classical mixed finite elements for a grid made up of rectangular solids to the deformed grid made up of hexahedra results in a method that is convergent only in case the hexahedra of the deformed grid are parallelepipeds. Several possibilities have been proposed for grids that are made up of true hexahedra with planar faces. However the deformations may lead to grids in which at least one side of some of the elements is non planar: for example the unit cube $[0,1]^3$ may be deformed by moving the two vertices $(0,0,1)$ and $(1,1,1)$ to $(0,0,2)$ and $(1,1,2)$ respectively. We propose a mixed finite element method that converges for grids made up of such "generalized hexahedra".

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MS50

Superconvergence for Control-volume Mixed Finite Element Methods on Rectangular and Quadrilateral Grids

Control-volume mixed finite element methods associate a control volume (covolume) with the vector variable as well as the scalar variable. In the context of flow in porous media, this yields a local Darcy law on the covolume associated with each discrete vector equation, in addition to the usual local mass conservation arising from the scalar equation on each grid cell. We formulate these methods on rectangular and distorted quadrilateral grids, and briefly discuss their relationships to some other locally conservative schemes that model flow on distorted grids. Exploiting a relationship to the lowest-order Raviart-Thomas mixed FEM, we demonstrate second-order superconvergence for the vector variable in a discrete $H(\text{div})$-norm and for the scalar variable in a discrete L^2-norm. In the quadrilateral case, this requires that the elements be second-order approximations of parallelograms as the mesh is refined.

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MS50

A Posteriori Error Estimation based on Potential and Flux Reconstruction for the Heat Equation: A Unified Framework

We derive a posteriori error estimates for the discretization of the heat equation in a unified setting comprising the discontinuous Galerkin, finite volume, and mixed finite element methods in space and the backward Euler scheme in time. Our estimates are based on a H^1-conforming potential reconstruction, continuous and piecewise affine in time, and a locally conservative $\mathbf{H}(\text{div})$-conforming flux reconstruction, piecewise constant in time. They yield a guaranteed upper bound. Local-in-time lower bounds are also derived.

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MS50

Iterative Coupling of Two-Phase Flow on General Hexahedral Grids

We present an iterative coupling method for the two-phase flow in porous media on the corner point geometry. The pressure equation is solved by the multipoint flux mixed finite element (MFMFE) method. Discontinuous Galerkin method is employed for the saturation equation. Numerical examples show the efficiency of this approach.

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MS51

A Model Predictive Controller Design for Parabolic PDE Systems

Abstract unavailable at time of publication.

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MS51

Model Reduction with Stability Guarantee for Linear and Nonlinear Systems Arising in Analog Circuit Applications

In this talk I present recently developed techniques for generating stable reduced models from linear and nonlinear systems arising in analog applications. These techniques combine the standard model reduction notions of projection and fitting along with convex optimization, and are capable of generating guaranteed stable reduced models from systems for which traditional algorithms are unreliable, such as when the original systems are highly nonlinear, described by unstructured and indefinite matrices, or even mildly unstable.

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MS51

On the Connection Between Model Reduction and N-Widths Approximation

The connection between two important model reduction techniques, namely balanced proper orthogonal decomposition (POD) and balanced truncation is investigated for infinite dimensional systems. In particular, balanced POD is shown to be optimal in the sense of distance minimization in a space of integral operators under the Hilbert-Schmidt norm. Whereas balanced truncation is shown to be a particular case of balanced POD for infinite dimensional systems for which the impulse response satisfies certain finite energy constraints. POD and balanced truncation are related to certain notions of metric complexity theory. In particular both are shown to minimize different n-widths of partial differential equation solutions including the Kolmogorov and Gelfand n-widths. The n-widths quantify inherent and representation errors due to lack of data and loss of information.

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MS51

A Thick-Restart Krylov Subspace Method for Order Reduction of Large-Scale Linear Descriptor Systems

In recent years, Krylov subspace techniques have proven to be powerful tools for order reduction of large-scale linear dynamical systems. The most widely-used algorithms employ explicit projection of the data matrices of the dynamical systems, using orthogonal bases of the Krylov subspaces. For truly large-scale systems, the generation and storage of such bases becomes prohibitive. In this talk, we explore the use of thick-restart Krylov subspace techniques to reduce the computational costs of explicit projection.

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MS51

Including Broadband Interactions and Boundary Forcing in Low and Least Order Galerkin Models of Fluid Flows

Abstract unavailable at time of publication.

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MS52

A Variant of Nonlinear Conjugate Gradient using

a Little Second-derivative Information

We propose an algorithm for minimization of unconstrained strongly convex functions that uses a small amount of second derivative information. It is based on Nemirovsky and Yudin's generalized conjugate gradient but appears to perform better in practice than their method and other variants of conjugate gradient. The method also extends to unconstrained nonconvex optimization.

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MS52

Accelerated Stochastic Approximation Methods for Composite Convex Minimization and Statistical Learning

In this talk, we present accelerated stochastic algorithms as well as novel accurate certificates for a few stochastic composite optimization problems including those involving strong convexity. We show that these algorithms are optimal in terms of expected rate of convergence, and also demonstrate that these convergence rates exhibit or can be improved so as to have a logarithmic dependence on a given reliability level. We demonstrate the significant advantages of these algorithms applied to statistical learning, such as the classic regression and support vector machine models.

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MS52

Primal-Dual First-Order Methods for a Class of Cone Programming

In this talk, we study first-order methods for a class of cone programming problems which, for example, include the MAXCUT semidefinite programming relaxation, Lovász capacity and those arising in compressed sensing. In particular, we first present four natural primal-dual smooth convex minimization reformulations for them, and then discuss first-order methods, especially a variant of Nesterov's smooth (VNS) method for solving these reformulations. The associated worst-case major arithmetic operation costs of the VNS method are estimated and compared. We conclude that the VNS method based on the last reformulation generally outperforms the others. Finally, as one example, we discuss the application of the VNS method to the Dantzig selector (DS) problem recently proposed by Candès and Tao, which has numerous applications in sparse signal recovery, variable selection and model fitting in linear regression. Though the DS problem can be reformulated and solved as a linear program, it is extremely challenging to the well-known methods such as simplex and interior point (IP) methods due to high dimensionality and full density of the data often encountered in practice. The performance of the VNS method is finally compared with the IP method that is tailored for the DS problem on a set of randomly generated instances. Our computational results demonstrate that while low-accuracy solutions are sought, the VNS method when applied to the most suitable reformulation mentioned above substantially outperforms the IP method that is superior to simplex methods.

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MS52

First-order Methods in Sparse Optimization

We discuss gradient-based methods in regularized logistic regression, compressed sensing, and support vector machines with kernel approximation. These sparse optimization problems are convex, involve simple nonsmooth functions, and have very high dimension in primal and/or dual space, with only a small fraction of the variables being nonzero at the solution. Such approaches as gradient sampling, nonstandard step lengths, and limited use of curvature information will be presented.

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MS53

Solving PDEs with RBFs: Applications in Geoscience Modeling

Radial basis functions have the advantage of being spectrally accurate for arbitrary node layouts in multiple dimensions with extreme algorithmic simplicity, and naturally permit local node refinement. We will show test examples ranging from vortex roll-ups, modeling idealized cyclogenesis, to unsteady nonlinear flows posed by the shallow water equations on a sphere to 3-D mantle convection in the earth's interior. Their performance will be evaluated based on numerical accuracy, stability and computational performance.

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MS53

Radial Basis Functions for Solving Partial Differential Equations

Compared to pseudospectral methods, radial basis functions (RBFs) have relinquished orthogonality properties in exchange for much improved simplicity and geometric flexibility, offering spectral accuracy together with local node refinement. A counterintuitive parameter range (making all the RBFs flat) is of special interest. Computational cost and numerical stability were initially seen as potential difficulties, but major progress have recently been made also in these areas.

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MS53

2D Radial Basis Function Interpolation on Irregular Geometry through Conformal Transplantation

Radial Basis Function (RBF) method for interpolating two dimensional functions with localized features defined on irregular domain is presented. RBF points are chosen such that they are the image of conformally mapped points on concentric circles on a unit disk. On the disk, fast RBF solver to compute RBF coefficients developed by Karageorghis et al. is used. Approximation values at desired points in the domain can be computed through the process of conformal transplantation.

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MS53

C-infinity Compactly Supported Radial Basis Function Methods for PDEs

Approximations based on analytic radial basis functions (RBFs), such as Gaussians and multiquadrics, are in many cases unstable when scattered nodes are used. On the other hand, methods based on RBFs of finite smoothness converge at algebraic rates even when the target function is smooth. Numerical experiments suggest that collocation methods based on C^∞ compactly supported radial basis functions are stable and yield exponential convergence. In this talk we explore the use of C^∞ RBFs for the solution of PDEs.

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MS54

K-12 Outreach with Integrated Math and Physics for Roller Coaster Design

We present an overview of learning experiences focused on roller coaster design that integrate mathematics and physics for grades 7-12. This workshop will include some hands-on design aspects and ideas that can easily be implemented in the classroom or as part of an after-school enrichment program. These projects are motivated in part by a NYSED funded school year program targeted at middle and high school students that culminates at a week long, roller coaster camp each summer and the use of a programmable Maxight 2002 Virtual Reality Roller Coaster that resides on our campus and a visit to Six Flags to collect data on real roller coasters.

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MS54

Soap and Slope: Exploration of Gradients through Hands-on Experiments with Surfactants (Outreach Module for Grades 7-12)

The purpose of this session is to share outreach activities used successfully with middle and high school students. I will demonstrate (and you can try!) activities to introduce the concept of slope (gradient) through activities with simple and inexpensive materials. We will also discuss how to tie outreach activities to discussions with students about research in applied mathematics.

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MS54

Applied Mathematics for High School Outreach

Contests can be a valuable motivator for introducing middle and high school students to applied mathematics. This talk will introduce some of the competitions that are available. Opportunities for both professional development and for student-based activities in applied mathematics will be presented. The talk will also provide a brief introduction to the remainder of the minisymposium.

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MS54

Computational Math, Science and Technology (C-MST) at K-12

An integrated (computational) approach to STEM education offers many benefits to improve teaching and learning at both college and secondary school classrooms. Computational thinking (CT) is now recognized as a fundamental skill to be taught along reading and writing. Our CT experience at K-12 shows a significant impact on student achievement in an urban school district. To sustain these experiences in K-12 classrooms, we need to improve technological pedagogical content knowledge (TPCK) of current and future teachers.

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MS55

On Non-singular Assembly Mode Change of Paral-

lel Manipulators

Non singular assembly mode change of parallel manipulators has been discussed for a while within the robotics community. This term means that a parallel robot can pass from one solution of direct or inverse kinematics into another without crossing a singularity. We will show that all generic planar 3-RPR parallel manipulators have this ability. Using geometric and algebraic properties of the singularity surface we will give a proof and extend the question to other manipulators.

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MS55
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS55
Managing Uncertainties in Kinematics

Uncertainty is an inherent feature of kinematics problems. Indeed geometrical modeling, that leads to the kinematic equations, involves physical parameters (e.g. link lengths) that are only known up to some bounded error. We will show how interval analysis allows one to determine the influence of these uncertainties on the kinematic performances. If this influence leads to unsatisfactory performances a variant of the analysis algorithm allows to determine almost all possible values for the physical parameters.

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MS55
Compliant Mechanism Analysis and Synthesis via Polynomial Solvers

This talk presents the use of polynomial solvers in the analysis and synthesis of compliant mechanisms. The motion of compliant mechanisms is governed by a set of kinetostatic (kinematics and statics) equations which can be transformed into a polynomial system. Solving these polynomial systems is one important step towards the innovative design of these compliant mechanisms. It has been found that a large portion of the solutions obtained by polynomial solvers have no physical meaning. Sifting out these mathematical solutions can be tedious even challenging in many cases. We also present a new technique called "constrained homotopy' technique for excluding unwanted solutions from a polynomial system.

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MS56
Fully Implicit Methods for Kinetic Simulation of Plasmas

We consider a fully implicit solution algorithm for the Vlasov-Poisson equation. By design, we employ the particle-in-cell (PIC) approach to describe kinetic populations. Algorithmically, we employ preconditioned Jacobian-free Newton-Krylov techniques to solve the resulting nonlinear systems. Our implicit PIC approach is unique in that it guarantees exact conservation of mass, momentum, and energy. Additionally, it is free from deleterious finite-grid (aliases) instabilities, which have imposed fundamental efficiency limitations in other PIC implementations.

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MS56
An Asymptotic Preserving Scheme for Kinetic Equations and Related Problems with Stiff Sources

Granular gases appear in various situations, such as dissipative diluted flows or pollen dispersion. Their mesoscopic description is given by the inelastic Boltzmann equation. We design numerical schemes to perform simulations on the evolution of the macroscopics quantities associated to this equation in different regimes. A numerical scheme for this equation might be able to deal both with the kinetic regime and its (stiff) hydrodynamic regime, obtained respectively when the mean free path goes to zero. Such a scheme is called Asymptotic Preserving (A.P.). In this talk we present a quasi-elastic model and the associated A.P. scheme, and compare the macroscopic quantities associated to this scheme with the ones obtained by Euler equations for dissipative gases. The technique used to derive the scheme is rather smooth and might be applied for a large class of problems, such as hyperbolic ones with relaxation or semiconductor equations.

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MS56
High Order Semilagrangian Methods for BGK and Vlasov Equations

In this talk we review some recent results on high order numerical schemes for some class of kinetic equations. We first describe high semilagrangian schemes for the BGK model of the Boltzmann equation. The schemes are based on writing the equation in characteristic form, and integrating it by high order diagonally implicit Runge-Kutta methods. The implicit treatment of the collision term allows the numerical solution of the equation even near the fluid dynamic regime. Peculiar property of the BGK equation are exploited to explicitly compute the implicit term. The semilagrangian nature of the scheme allows the use of large time steps, overcoming the usual CFL limitation. High order in space is obtained by suitable high order

WENO reconstruction. A recently developed conservative version of the scheme is proposed. A similar scheme is applied to the solution of the BGK equation in a domain with moving boundary. The equation is solved on a fixed grid. The solution is computed on the grid points inside the domain, which change in time. Boundary conditions are satisfied by suitably defined ghost values on grid points near the boundary, in the exterior of the domain. As a last application, new high order semilagrangian methods for the Vlasov equation will be presented. The method is based on writing the equation in characteristic form. At each grid node in space and velocity, the characteristics are traced back in time, and the value at the foot of the characteristics are computed by high order WENO reconstruction. Preliminary results show the effectivenes of the approach.

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MS57

Characterization of Discontinuities in High-dimensional Stochastic Problems on Adaptive Sparse Grids

The behavior of financial, chemical, mechanical, environmental and many other processes are often characterized by a large number of variables. The relationship between the variables that drive the system (inputs) and the system response (outputs) can be highly non-linear, discontinuous and correlated. Knowledge of the relationships between the model inputs and outputs can be extremely useful when attempting to quantify uncertainty, construct surrogate models or evaluate high-dimensional integrals. This talk presents a numerical procedure for determining jump discontinuities in high dimensional functions on sparse adaptive grids. This method combines the strength of dimension adaptive sparse grid approximation and polynomial annihilation edge detections to construct a high order method, which provides easy and effcient detection of jump discontinuities in highly variable functions.

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MS57

Wave Scattering by Randomly Shaped Objects

Abstract not available at time of publication.

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MS57

Non-intrusive Polynomial Chaos Application to Acoustic Rough Surface Scattering

A computational inverse Riemann map allows acoustic modeling of rough sea surface scattering by sound speed variations in the Helmholtz equation with flat surface. Use of a standard underwater acoustic propagation model with the resulting sound speeds provides the basis for non-intrusive polynomial chaos calculations. Applications include typical acoustic field variability measures. This research is sponsored by the Office of Naval Research.

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MS57

Uncertainty Quantification Methodologies for Climate Model Data with Discontinuities

Uncertainty quantification in climate models is challenged by the sparsity and bifurcative character of the available climate data. To circumvent these challenges we propose a methodology that employs Bayesian inference to locate discontinuities in the model output, followed by an efficient propagation of uncertain quantities using spectral expansions of random parameters/fields. Stochastic emulators are used to assess the performance of the proposed approach.

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MS58

Decreasing of the Perimeter under Generalized Steiner Symmetrization and Characterization of Cases of Equality

Abstract not available at time of publication.

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MS58

Variational Approaches to Bar Code Reconstruction

In this talk we will discuss TV-based energy minimization for deblurring and denoising of 1D and 2D bar codes. For 1D bar codes, we consider functionals consisting of the TV-seminorm together with various fidelity terms involving deconvolution and a convoluted signal of a barcode. Key length scales and parameters are the X-dimension of the bar code, the sizes of the supports of the convolution and deconvolution kernels, and the fidelity parameter. For these functionals we establish parameter regimes (sufficient conditions) wherein the underlying barcode is the unique minimizer. We present some numerical experiments experiments which suggest that these sufficient conditions are not optimal, and the energy methods are quite robust for significant blurring. For 2D barcodes, we discuss minimization of a functional comprised of an anisotropic TV norm and an L^1 fidelity term. We present necessary and sufficient conditions for a minimizer and apply our results to denoising and deblurring of 2D bar codes. We also present numerical experiments.

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MS58

Stability in the Wulff Inequality and Applications

The equilibrium shape of a crystal is determined by the minimization under a volume constraint of its free energy, consisting of an anisotropic interfacial surface energy plus a bulk potential energy. In the absence of the potential term, the equilibrium shape can be directly characterized in terms of the surface tension and turns out to be a convex set, the Wulff shape of the crystal. Our first result is a sharp quantitative inequality implying that any shape with almost-optimal surface energy is close in the proper sense to the Wulff shape. This is a joint work with Francesco Maggi (Florence) and Aldo Pratelli (Pavia). Under the action of a weak potential or, equivalently, if the total mass of the crystal is small enough, the surface energy of the equilibrium shape is actually close to that of the corresponding Wulff shape, and the previous result applies. However, stronger geometric properties are now expected, due to the fact that the considered shapes are minimizers. Indeed we can prove their convexity, as well as their proximity to the Wulff shape with respect to a stronger notion of distance. This is a joint work with Francesco Maggi (Florence).

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MS58

A Hierarchy of Elastic Plate Models with Residual Stress

Abstract not available at time of publication.

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MS59

Using Homotopy Continuation to Quickly and Accurately Solve Polynomial Systems

Homotopy continuation solves any size polynomial system of equations, but as the number of variables rise, so do complications and computation time. Since the systems may be unsolvable by hand, it is hard to obtain an accurate count of how many solutions there are. Poor approximations cause lengthy calculation due to evaluating diverging homotopy paths. By eliminating these early, we can cut computation time and devote resources to accurately tracking the roots.

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MS59

Numerical Simulation of a Brownian Elastic Filament in Random Stokes Flow

The dynamics of elastic filaments in Stokes flow has significant effects on their ability to be transported. We numerically investigate the dynamics of an elastic filament in a random Stokes flow using Tonberg and Shelley algorithm. This includes the filament susceptibility to buckling instability, and its effective diffusivity. Furthermore, thermal fluctuations are incorporated, and their effects on filament transport in Stokes flows are quantified. Finally, preliminary work on the hydrodynamic interaction effects on filament transport will be presented.

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MS59

Adaptive Hybrid Trigonometric Polynomial Reconstructions

Fourier series approximations have difficulties with discontinuous functions. Our approach to remedy this problem is to use a hybrid method. In this method, polynomial approximation is used near the discontinuity and Fourier approximations are used on the other regions. We present numerical differences between our methods and other previous methods applied to similar popular problems. Moreover, we attempt to reduce the error caused by aliasing.

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MS59

Distributed Compressive Imaging

Compressive imaging offers the possibility of completely new imaging sensor design which can dramatically reduce the sampling rates currently required for perfect image reconstruction. Distributed Compressive Imaging (DCI) offers a type of joint image compression/reconstruction of imaging sensors which have overlapping fields-of-view. We formulate the mathematical model of the sensing network in terms of distributed compressive sensing and simulate the image reconstruction results over a variety of sensor configurations and a priori knowledge.

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MS59

Jump Discontinuity Detection with Noisy Fourier Data

The detection of jump discontinuities in physical space using frequency (Fourier) data is an essential aspect of Medical Resonance Image processing. The difficulty of the task lies in extracting local information from the global Fourier data, and is further complicated by noise. In this talk, we discuss a recently developed algorithm that uses frequency data to recover the jump discontinuities. The expected accuracy of the detector has been modeled using statistical hypothesis testing.

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MS59

High-Order Adaptive Methods for Drawing Parametric Curves

A naive way to draw a parametric curve is to plot a finite number of equally spaced parameter values and interpolate them with lines. Linear interpolation has low accuracy, especially near points of high curvature and uniformly spaced points over-resolve some parts of a curve while under-resolving others. We develop a method that places the points adaptively and interpolates them with higher-order interpolants called Catmull Rom Spline–piecewise Bezier Curves. We validate this with numerical experiments.

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MS60

Stochastic Modeling of Parasites in Host Populations

The complexity of the host-parasite relationship, and its depression of host populations has been investigated and successfully modeled for large populations using deterministic methods. These models fail to accurately predict interactions within smaller populations, and require a statistical component to reclaim some degree of accuracy. This research employs stochastic differential equations to better forecast changes in small populations, and, in a practical setting, seeks to write software that will automate this procedure.

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MS60

Mathematical Models for Predicting Survival and Internal pH for Food Pathogens

The risk of disease outbreaks from acidified vegetable products due to microbial pathogens such as Escherichia coli (E. coli) O157:H7 is of recent concern. For conditions similar to these products, we developed a mechanistic model describing the internal pH of E. coli. In addition, a Weibull model was used to relate survival to internal pH and experimental methods were implemented to validate model predictions. Our efforts may result in improved methods for inactivating these pathogens.

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MS60

Mathematical Models of Interneurons in Hippocampus

The hippocampus is an intensely studied brain structure that is involved in learning and memory. It expresses several population activities that are controlled by a diverse collection of inhibitory cells, or interneurons. These interneurons have distinct characteristics that can contribute to network output in different ways. I will describe our work involving the development and analysis of detailed models of hippocampal interneurons so as to help understand the contribution of their distinct natures.

Frances Skinner
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MS60

Boolean Models Can Explain Bistability in the Lac Operon

The lac operon is a well-studied gene system known to exhibit bistability. While most models are based on complex functions, it has been suggested that specifiying network topology is sufficient to capture dynamics. We present a Boolean model and show that it accurately reproduces the operon's dynamics. Further we identify a core subnetwork that maintains bistability. These results support the hypothesis that topology is the key to model qualitative dynamics in gene systems.

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MS61

Better Methods Through Optimization, Or How to Avoid Doing the Hard Work Yourself

We use optimization and control ideas to formulate better numerical methods for PDEs. Two applications are presented: an additive decomposition approach for coupled multi-physics problems, and bounds preserving remap algorithm. In the first case, we synthesize scalable solvers for advection-dominated PDEs that work for all Peclet numbers from standard AMG solvers that fail in the advection dominated regime. In the second case, we derive a compatible transport algorithm that ensures monotonicity of a tracer.

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MS61

Coarse-scale Models for Flows in High-contrast Multiscale Media and their Applications

In this talk, I will discuss special coarse spaces for multiscale finite element and domain decomposition methods. These spaces allow a coarse-scale representation of the solution of multiscale flow problem. The focus will be on problems that have high variations in the media properties. It is known that the number of iterations in domain decomposition and many iterative methods is adversely affected by the contrast in the media properties. One way to decrease the number of iterations is to choose coarse spaces appropriately. In the proposed methods, the coarse spaces are constructed based on a local eigenvalue problem. We show that if domain decomposition methods use these coarse spaces then the condition number of preconditioned system is independent of the contrast in media properties. The coarse space can have large dimension. In this talk, we discuss dimension reduction for the proposed coarse spaces and hierarchical computations of multiscale basis functions. The latter results to domain decomposition preconditioners that have the condition number which is independent of contrast. We will discuss the accuracy of coarse-scale solutions using these proposed coarse spaces. Numerical results will be presented.

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MS61

Iterative Algorithms based on the Algebraic Multiscale Finite Volume Method

In the Multiscale Finite-Volume (MsFV) method a conservative velocity field is constructed from an approximate pressure field, which is obtained by juxtapposition of local solutions coupled through a global problem. Due to localization assumption, the MsFV solution differs from the exact solution of the problem. The accuracy of the method can be improved by constructing an iterative algorithm that arbitrarily reduces the localization error. We present these iterative algorithms and several applications.

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MS61

Domain Decomposition for Poroelasticity and Elasticity with DG Jumps and Mortars

A nonoverlapping mortar domain decomposition algorithm is formulated for a poroelastic payzone region coupled with an elastic non-payzone region. A continuous Galerkin method is used for the displacement variables and the interface operator is constructed using discontinuous Galerkin jump conditions. Optimal order error estimates are presented, as well as a multiscale algorithm which increases the computational efficiency. Numerical results are presented for a 2D example with an analytic solution and a more complicated 3D example.

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MS62

Scenario Discovery Using Nonnegative Tensor Factorization and Visual Analytics

Automated approaches for the identification and clustering of semantic features or topics are highly desired for text mining applications. Moving beyond two-way factorizations, we demonstrate how non-negative tensor factorizations (NNTFs) can be used to capture temporal and semantic proximity for tracking targeted and latent discussions. Visualization of NNTF outputs for topic detection and tracking using email corpora from Enron and the Climate Research Unit (CRU) at the University of East Anglia is demonstrated.

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MS62

Sparse Optimization with Least-squares Constraints

The use of convex optimization for the recovery of sparse signals from incomplete or compressed data is now common practice. Motivated by the success of basis pursuit in recovering sparse vectors, new formulations have been proposed that take advantage of different types of sparsity. We propose an efficient algorithm for solving a general class of sparsifying formulations. For several common types of sparsity we provide applications, along with details on how to apply the algorithm.

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MS62

Generalizations of Subspace Identification for Learning from High-Dimensional Time Series Data

Kalman filters and HMMs are staples for analyzing time series data. Factor analysis methods (such as PCA) are staples for analyzing high-dimensional data. In the linear-Gaussian case, subspace identification methods have brought together these two model classes to analyze high-dimensional time-series data. Recently, researchers have begun to generalize subspace ID beyond linear-Gaussian models, to handle representations such as HMMs. I will discuss our work in this direction, using examples and results from robot sensor data.

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MS62

Nonnegative Matrix Factorization using Bicliques

Nonnegative matrix factorization is an important data mining technique, with applications in genomics, the natural sciences, and information retrieval. These are usually recovered using optimization techniques requiring dense representation of the factors, which sharply limits the number of rank-one components we can identify; a problem because of the fat-tail (power-law) distribution of those components. We demonstrate how to use biclique enumeration algorithms to obtain much more complete factorizations, and show results on some real datasets.

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MS63

Domain Decomposition Methods for Stokes-Darcy Systems with Boundary Integrals

We consider a coupled problem of Stokes and Darcy equations. This involves solving PDEs of different orders simultaneously. To overcome this difficulty, we apply a non-overlapping domain decomposition method based on Robin boundary condition obtained by combining the velocity and pressure interface conditions. The coupled system is then reduced to solving each problem separately by an iterative procedure using a Krylov subspace method. The numerical solution in each subdomain is based on boundary integral equation.

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MS63

Regularization Methods for Biological Fluid Flow Problems

Biological flows surrounding swimming microorganisms or beating cilia are modeled using the Stokes equations with external forcing. The organism surfaces are flexible interfaces imparting force or torque on the fluid. I will present recent advances of the Method of Regularized Stokeslets, which is based on integral expressions for the exact fluid velocity field resulting from localized regularized forces. I will present the idea of the method, some of the known results and several examples from biological applications.

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MS63

A Non-stiff Boundary Integral Method for 3D Porous Media Flow with Surface Tension

An efficient, non-stiff boundary integral method for 3D porous media flow with surface tension is presented. Surface tension introduces high order (i.e., high derivative) terms into the evolution equations, and this leads to severe stability constraints for explicit time-integration methods. Furthermore, the high order terms appear in nonlocal operators, making the application of implicit methods difficult. Our algorithm employs a special representation of the interface which enables efficient application of implicit time-integration methods via a small-scale decomposition. The algorithm is found to be effective at eliminating the severe time-step constraint that plagues explicit time-integration methods.

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MS63

Solution of Coupled Free/porous Media Flow using Boundary Integral Equations

Fluids partly flowing freely and partly filtrating through a porous medium are modeled by a coupled Stokes-Darcy system with carefully chosen interface conditions. In this talk, we describe a boundary integral formulation for this problem, where the Green's function is regularized and correction terms are added for higher accuracy. A preconditioner based on the regularization-correction method is developed to improve the convergence of a Krylov subspace method to solve the integral formulation.

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MS64

Geometry of Sums of Squares Relaxations

Lasserre relaxations are a very common optimization tool to approximate semi-algebraic sets by projections of spectrahedra. In this talk we will revisit a result of Netzer, Plaumann and Schweighofer on the geometry of these sets and present a more elementary proof for it. We will then procceed to do a few extensions of this result and solve some related open questions.

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MS64

Geometry of Restricted Boltzmann Machines

The restricted Boltzmann machine is a graphical model for binary random variables. Based on a complete bipartite graph separating hidden and observed variables, it is the binary analog to the factor analysis model. We study this graphical model from the perspectives of algebraic statistics and tropical geometry, starting with the observation that its Zariski closure is a Hadamard power of the first secant variety of the Segre variety of projective lines. We derive a dimension formula for the tropicalized model, and we use it to show that the restricted Boltzmann machine is identifiable in many cases. Our methods include coding theory and geometry of linear threshold functions.

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MS64

Semidefinite Representations for Orbitopes

Orbitopes are highly symmetric convex bodies obtained by taking the convex hull of an orbit of a compact group acting linearly on a real vector space. For linear algebraic groups and rational representations, the orbit is a real variety and thus the orbitope can be approximated by projections of spectrahedra via Lasserre's moment relaxation. We show that the level at which the relaxation is exact can often be analysed based on simpler objects and in some case be determined exactly by studying the geometry of certain associated polytopes. We will discuss this method on several well known examples of orbitopes and show how an old conjecture by Harvey and Lawson appears in new light, when discussed in this context. If time permits we will discuss first steps towards the resolution of this conjecture in particular cases as well as convincing evidence using numerical algebraic geometry.

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MS64

Convex Algebraic Geometry

Convex algebraic geometry, which is the study of convex semi-algebraic sets, is a discipline that arose from optimization, specifically semidefinite programming and polynomial optimization. It seeks to develop algorithms and software to treat convex sets defined by algebraic equations and inequalities, as well as to better understand such sets, and exploit this understanding in applications, from optimization to algebraic statistics to control. This minisymposium will present current work in this new field from foundational material to applications and algorithms.

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MS65

Promoting Professional Development for Undergraduates Through Calculus Projects

We present projects used in Freshmen Calculus I and II courses that promote professional development at a very early phase of undergraduate education. We focus on some that are based on designing a safe and thrilling roller coaster. Students integrate Mathematics and Physics in their analysis with a strong emphasis on technical communication throughout. We discuss extensions to other courses and our experiences in managing projects in large lecture sections with more than 100 students.

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MS65

Career Preparation of Undergraduate and Graduate Students through an Interdisciplinary Consulting Approach

It is vital for Mathematicians and Statisticians to interact effectively with colleagues from other fields. We have implemented a training approach through consulting with clients from application areas to provide our students with demonstrated experience of their skills in this area. On the graduate level, we use a consulting center, and on the undergraduate level, we have created an REU Site using the same philosophy. This talk will show both the ideas and their implementation in more detail.

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MS65

Career Training Opportunities at the University of Tennessee

Opportunities at the University of Tennessee and the National Institute for Mathematical and Biological Synthesis will be presented. Unique training programs through new graduate fellowship grants will be discussed. Our REU and REV (research experiences for veterinary students) summer program and the institute postdoc program will be highlighted.

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MS65

The Applied Mathematics & Statistics, and Scientific Computation Program (AMSC) at the University of Maryland: Interdisciplinary Research in a Flexible and Structured Environment

Abstract unavailable at time of publication.

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MS66

Interaction of Elastic Biological Structures with Complex Fluids

Often, biological fluids are non-Newtonian and exhibit viscoelastic responses. We will present recent progress on the development of computational models of pumping and swimming in a viscoelastic fluid. An immersed boundary framework is used, with the complex fluid represented by a continuum Oldroyd-B model.

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MS66

Mechano-Chemical Models of Ionic Effects in the Cellular Microenvironment of Articular Cartilage

Articular cartilage extracellular matrix (ECM) is comprised of collagen fibers and proteoglycan macromolecules. Proteoglycans have a net negative charge, giving rise to a fixed charge density that couples with ions dissolved in the interstitial fluid to alter tissue mechanical properties with fluid osmolarity. In this talk, I will present models for quantifying the contribution of fixed charge density to ECM stiffness in the microenviroment of cartilage cells based on the use of triphasic (fluid-solid-ion) continuum mixture theory.

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MS66

A Multi-scale Model for Polymer-laden Flows Coupling Stochastic Particle Dynamics with Continuum Fluid Mechanics

Polymer-laden flows exhibit complex rheology, especially on length scales comparable to individual extended macromolecules. Such flows occur in biological systems and in microfluidic devices. To simulate these problems we have developed an efficient and stable kinetic method, which couples constrained stochastic particle dynamics with an incompressible second-order accurate Navier-Stokes solver. The algorithm is based Kramers' bead-rod approximation of a polymer, with a reverse coupling approximated via a discrete (cloud-in-cell) delta function. The constrained particle dynamics are expressed as a system of stochastic ODEs with explicit Lagrange multipliers, and discretized with a second-order Ito-Taylor expansion. By itself, this particle method is second-order accurate in both strong and weak senses. To make the particle method stable with fluid CFL-limited time steps, we use a Duhamel formulation of the dynamics. The Navier-Stokes continuum solver is based on a second-order projection method with the embedded boundary technique to represent complex fluid domains.

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MS66

Multiphase Mixture Modeling of Microbial Biofilms

Much of the earth's microbial biomass resides in sessile, spatially structured biofilms consisting of large numbers of single celled organisms living within self-secreted biologically and chemically active viscoelastic matrices made of polymers and other molecules, with important consequences to both form and function. Here we present a multiphase mixture model including physical (e.g. mechanics), chemical (e.g. mineral precipitation), and biological (e.g. growth) components, and discuss implications.

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MS67

Exploiting Group Theory in Spectral Methods for PDEs

By exploiting symmetry, the cost of two-dimensional interpolation and/or summation by Legendre polynomials can be reduced by a factor of 3/2 (for large N) compared to transforms that exploit only the double parity symmetry of the square. In three dimensions, the savings is a factor of 18/5. These group-theory based tricks are valuable in high order spectral elements. We also explain how group symmetry can be exploited in collocation discretizations of PDEs when only the domain has symmetry.

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MS67

Automatic Fréchet Differentiation for the Spectral Solution of Boundary-value Problems

To solve a nonlinear BVP, a Newton iteration solves for corrections obtained through a Fréchet derivative, analogous to a Jacobian matrix. Automatic differentiation techniques are applied to compute the Fréchet derivative from a coded expression in the chebfun software system, a Matlab package that represents functions and operators using Chebyshev expansions and collocation. Thus, one can solve BVPs with automatic spectral methods, requiring only natural expressions of the equation and boundary conditions.

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MS67

Polynomial Chaos Methods for Differential Equations with Singular Sources

Singular sources represented by the Dirac δ-function in differential equations play a crucial role in determining the global solution. Physical parameters associated with the δ-function are highly sensitive to measurement errors. Polynomial chaos methods are used for the uncertainty analysis with uncertainties in location and strength of the δ-function for steady and time-dependent PDEs. The direct collocation projection method is also used to deal with the Gibbs phenomenon.

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MS67

Efficient, Energy-stable and Convergent Finite Difference Schemes for the Phase-field Crystal and Modified Phase-field Crystal Equations

We present unconditionally energy stable finite difference schemes for the phase-field crystal (PFC) and modified phase-field crystal (MPFC) equations. The methods are based on a convex splitting of a discrete energy and are semi-implicit. The equation at the implicit level is nonlinear but represents the gradient of a strictly convex function and is uniquely solveable regardless of the time step size. By controlling the energy, the stability of the scheme is guaranteed and local-in-time error estimates can be used to prove convergence of the schemes. We solve the nonlinear equations at the implicit time level using an efficient nonlinear multigrid. Numerical simulations are presented that confirm the stability, efficiency and accuracy of the schemes.

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MS68

Convex Relaxation for the Planted Cluster Problem

It is well-known that the problem of finding the maximum set of vertices comprised of k disjoint cliques of a graph, called a k-clique subgraph, is NP-hard. This problem can be formulated as a semidefinite program subject to a rank constraint. In the special case that the input contains a single large k-clique subgraph obscured by diversionary edges and nodes, this hidden structure can be recovered efficiently by solving the convex optimization problem obtained by relaxing rank with the nuclear norm. We provide two analyses when our algorithm succeeds. In the first, the diversionary edges are placed by an adversary. In the second, they are placed at random.

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MS68

Guranteed Rank Minimization with Singular Value Projection

Minimizing the rank of a matrix subject to affine constraints is a fundamental problem with many important applications in machine learning and statistics. In this talk we present a simple and fast algorithm SVP (Singular Value Projection) for rank minimization with affine constraints (ARMP) and show that SVP recovers the minimum rank solution for affine constraints that satisfy the restricted isometry property (RIP). We show robustness of our method to noise and prove a geometric convergence rate even for noisy measurements. Our method is simple to analyze and easier to implement in comparison to the recent trace norm based methods of Recht, Fazel and Parillo and Lee and Bresler. We also improve the existing RIP recovery results and achieve exact recovery under strictly weaker assumptions on the RIP constants than previously known.

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MS68

On Reweighted Trace Minimization for Low-rank Matrix Recovery

The problem of recovering a low-rank matrix consistent with noisy linear measurements is a fundamental problem with applications in machine learning, statistics, and control. Reweighted trace minimization, which extends and improves upon the popular nuclear norm heuristic, has been used as an iterative heuristic for this problem. We present theoretical guarantees for the reweighted trace heuristic. We quantify its improvement over nuclear norm minimization by proving tighter bounds on the recovery error for low-rank matrices with noisy measurements. Our analysis is based on the Restricted Isometry Property (RIP). Along the way we also improve the existing RIP recovery conditions for the nuclear norm heuristic, showing that recovery happens under a weaker assumption on the RIP constants.

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MS68

Title Not Available at Time of Publication

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MS69

The Turbulent Cascade of Entropy in Kinetic Simulations of Plasma Turbulence

Abstract not available at time of publication.

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MS69

Peta-scale Full Facility Linear Radiation Transport Calculations for Shielding Analysis.

Abstract not available at time of publication.

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MS69

High Order Split Integral Deferred Correction Methods for Vlasov Equations

We present arbitrary order time integration methods and their application to the Vlasov equations within a semi-Lagrangian framework. These integral deferred correction (IDC) methods solve an error equation to improve Strang splitting error beyond second order. We discuss benefits and limitations of higher order split time integrators obtained with the IDC framework in a semi-Lagrangian setting. Principles in this work can be extended to other operators suitable for splitting methods, such as Maxwell's equations.

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MS69

Finite Element Methods for Regularized 13-Moment-Equations

This talk discusses numerical methods for the linearized regularized 13-moment equations (R13) based on finite elements. The R13 equations have been derived from kinetic gas theory to model non-equilibrium gas flows. In linearized steady form these equations can be viewed as an extended version of the Stokes equation. We will present analytical solutions for the flow past a sphere and investigate variational formulations to be used in a finite element discretization. The software package FEniCS allows us to experiment easily with different formulations.

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MS70

Wave Propagation in Random Polycrystals

Abstract not available at time of publication.

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MS70

UQ for Fluid Mixing

New results are presented for several stochastic fluid mixing problems: turbulent Rayleigh-Taylor and Richtmyer Meshkov flows, primary breakup of a high speed jet and fluid mixing for chemical processing. We present the fluctuations associated with variation across an ensemble of spatially averaged quantities.In some cases, the experiments do not fully characterize the flow. In addition to obtaining experimental agreement (validation) with the simulations, we study the uncertainties associated with the actual experimental data (UQ).

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MS70
Accelerated Optimal Bayesian Experimental Design for Nonlinear Problems

The optimal selection of experimental conditions is essential to maximizing the value of data for both inference and prediction. We propose a general Bayesian framework for optimal experimental design with nonlinear simulation-based models. The formulation fully accounts for uncertainty in model parameters, experimental conditions, and observables. Straightforward evaluation of the objective function—which reflects expected information gain due to an experiment—is computationally intractable. Instead, the present construction relies on (i) polynomial chaos expansions, which capture the dependence of observables on uncertain model parameters *and* design conditions; and (ii) efficient stochastic optimization methods to maximize expected utility. We demonstrate these methods on stiff nonlinear chemical kinetic systems.

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MS70
Uncertainty Quantification for Sparse Random PDEs

An approach for quantifying parametric uncertainty in a stochastic model output is presented. It relies on pointwise evaluations of the output response surface. If the stochastic model output has a reasonably sparse representation in the retained approximation basis, the method retrieves the dominant modes of the solution approximation from a minimal number of evaluations. The methodology is applied to the solution of a 8-D stochastic Shallow Water problem and is shown to perform well.

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MS71
Comparison of Treatment Approaches in Alcohol Epidemiology

This talk considers the spread of alcohol abuse through a social network model accounting for peer influence and innate characteristics. The efficacy of several treatment approaches in reducing the prevalence of alcohol abuse is considered in scenarios where the individuals may generally be non-compliant towards treatment. Specifically, we compare a treatment program that targets the most problematic drinkers to a program that targets the most compliant individuals.

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MS71
Approximation of Detailed Hodgkin-Huxley-Type Neuronal Models by Exponential Integrate-and-Fire Models

Using current-voltage curves and spike metrics, optimal strategies are developed for finding the parameters in the exponential integrate-and-fire point neuron model with adaptation current that give the best approximation to the membrane potential and firing rate dynamics of a corresponding Hodgkin-Huxley-type model. The adaptation current is modeled explicitly, but has a prescribed jump at each spike time. The results of computations using both systems give excellent agreement. Bifurcations in both models are compared.

Dan Johnson
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tba

MS71
A Comparative Examination of CUDA and OpenCL for a Gravitational Wave Source Modelling Application

As CPU clock speeds stall out around 3 GHz, multicore systems are used to increase performance. But they have limitations (power consumption, heat dissipation). By making use of GPU programming languages (OpenCL, CUDA), one can harness the power of hardware already contained in a desktop system, and obtain over an order of magnitude gains in performance. In my work I will apply these aforementioned programming techniques to illustrate their power in a Gravitational Wave Source Modelling Application.

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MS71
Nonlinear Waves and Delay in Modeling Spiking Neurons

Synaptic delay plays a key role in understanding neurological disorders including Alzheimer's and Parkinson's diseases. In our work we model synaptic plasticity with delay equations. Specifically, we incorporate delay in a nonlinear wave equation to study conduction velocities and their dependence on timing between neural spikes, and determine phase and group velocities. We compare the computed results with available experimental data. In addition, we study interaction of two waves moving along an axon with

time overlap.

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MS72

Adjoint Models in Sensitivity Analysis and Predictability

Adjoint models are an important tool for sensitivity analysis and targeting strategies in variational data assimilation. We will discuss the use of first- and second-order adjoint models for sensitivity analysis and targeting strategies. A novel observation-targeting approach based on the second-order adjoint (SOA) model, to account for quadratic error growth, will be presented. The performance and reliability of the SOA targeting strategy is compared with more traditional strategies through experiments with a two-dimensional shallow-water model.

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MS72

Parameter Estimation in Stochastic Equations That are Second-Order in Time

Consider the following problems: 1. Given an undamped harmonic oscillator driven by additive Gaussian white noise, estimate oscillator's frequency from the observations of the oscillations; 2. Given an undamped wave equation driven by additive space-time white noise, estimate the propagation speed from the observations of the solution. It turns out that the the first (one-dimensional) problem is not necessarily easier to study than the second (infinite-dimensional) problem. The objective of the talk is to describe the asymptotic properties of the maximum likelihood estimator in both problems and to discuss various generalizations.

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MS72

Uncertainty Quantification (uq) for Component-Level Power System Models

The goal of the paper is for uncertainty quantification (UQ) of component level power system models, which can provide an error bar on component level modeling of power systems. Procedures include: Identify the most sensitive uncertain parameters; Represent these parameters with the given distributions; Generate probabilistic collocation points in the random parameter space; Perform simulations for each realization (sampling point set); Post-process the outputs and obtain the statistical results of the outputs.

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MS72

Comparison of Several Computational Methods for Variable Subset Selection

In this talk we report on an investigation of several computational methods for variable subset selection which is an important element for quantifying uncertainties in complex systems. The methods considered are: (1) correlation analysis using the method of Spearman, (2) the Morris screening method, (3) a modified Delta test, (4) the approximate model method based on the multivariate adaptive regression splines, and (5) sum-of-trees methods. Our contributions in this study are modifications made to some of these methods for enhanced robustness in variable selection as well as a numerical study of the effectiveness of these methods.

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MS73

Reflected Waves in Nonlocally Coupled Neural Networks

Recent experimental results show that propagation of waves between two different regions in the visual part of the brain lead to compression and sometimes reflection of the waves. The experimentalists suggest that this may be due to a change in the degree of inhibition. We show that this is unlikely and that a better explanation is a change in excitability. Analytic and numerical calculations back up our assertion.

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MS73

Generalized Sensitivity Functions for Delay Differential Equations

Delay differential equations are useful to model various biological processes in which there are hysteretic effects. A popular example is Hutchinson's equation, also known as the delay-logistic equation. We use this example to determine the effect of a delay on generalized sensitivity functions (which provide insight on sensitivity of estimated parameters to data). We compare the numerical approximations of the generalized sensitivity functions for the delay-logistic equation to the equation without delay.

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MS73

Mathematical Approach to Modeling the Effects of Ocean Acidification On the Pteropod and Pink Salmon Population

Ocean acidification is an extension of increased atmospheric CO2 content. One species greatly affected by ocean acidification are euthecosomatous pteropods, which may suffer shell and skeleton deterioration and growth delay. Furthermore, the pink salmon population in the North Pacific, targeted by commercial fisheries, have been known to prey heavily on pteropods. A discrete stage-structured model is developed to model the dynamics of this interaction in the wake of ocean acidification.

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MS73

Data Assimilation Study using a Simple Atmosphere-Ocean Model

The coupled ocean-atmosphere system has instabilities that span time scales from a few minutes to years. It is not clear whether data assimilation focused on long-term variability should include the smaller time scales, since the faster scales distort the slower longer time-scale solution. To study this problem, we employ two data assimilation schemes onto a simple nonlinear chaotic model of fast and slow versions of the Lorenz (1963) model with different strengths of coupling.

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MS74

Application of Datamining in Analyzing Large-Scale Network Evolution

Analysis of large-scale networks, such as social and biological systems, is extensively used to understand their characteristics and temporal evolution. However, most analysis algorithms do not take into account the properties of the underlying applications. In this talk we will discuss how data mining can be used to classify networks based on their properties and use this information to predict whether there will be significant modifications to the community structure, under addition or deletion of certain edges.

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MS74

Large, Sparse Network Alignment Problems and a New Algorithm

Network alignment is a standard problem in data mining and bioinformatics. We begin by comparing a network from Wikipedia with one from the Library of Congress. We describe a unified mathematical framework for network alignment solvers, a sparse variant of the problem, and a new algorithm based on a message passing or belief propagation heuristic. This algorithm is fast – running in minutes on graphs with over 1000000 edges. Our codes are available online: http://www.stanford.edu/ dgleich/publications/2009/netalign/index.html.

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MS74

Predictive Modeling for Relational and Network Domains

Recently there has been a surge of interest in methods for analyzing complex social networks (e.g., communication and friendship networks). For predictive modeling, the dependencies among linked entities in the networks present an opportunity to improve inference about properties of individuals. This presentation will outline the characteristics of network data that differentiate it from the traditional settings for inference and learning, and discuss specific techniques for incorporating relational information into statistical models and algorithms.

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MS74

Clustered Embedding of Massive Online Social Networks

In this talk we will describe a novel technique called *clustered spectral graph embedding*, to capture fundamental structure in social network graphs. The proposed procedure is an effective and highly scalable tool for various tasks in computational analysis of social networks. We will demonstrate our approach to (1) approximate proximity measures and (2) predict new friendship links using three very large real-world social network data sets: Flickr, Live-Journal and MySpace.

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MS75

A Cartesian Grid Method For Two-phase Gel Dynamics on an Irregular Domain

We develop a numerical method for simulating models of two-phase gel dynamics in an irregular domain using a regular Cartesian grid. Multigrid with Vanka-type box relaxation scheme is used as preconditioner for the Krylov subspace solver to solve the momentum and incompressibility equations. Ghost points are used to enforce the boundary conditions. The behavior of the new method is explored through numerical experiments for a problem with strong phase separations.

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MS75

Computation of Porous Media Flows using Octree Adaptive Mesh Refinement

In this talk I will describe a novel approach for the simulation of two-phase flows in porous medium. This approach makes use a a newly devised framework for solving partial differential equations on Octree adaptive grids. A hallmark of this approach is that non graded adaptive grids can be used and boundary conditions are imposed implicitly, which avoids the difficulties associated with remeshing. Examples of such simulations will be presented.

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MS75

Simulating Biochemical Signaling Networks in Complex Moving Geometries

Signaling networks regulate cellular responses to environmental stimuli through cascades of protein interactions. External signals can trigger cells to polarize and move in a specific direction and maintain spatially localized activity of proteins. To investigate the effects of morphological changes on intracellular signaling, we present a numerical scheme consisting of a cut cell finite volume discretization coupled with level set methods. This method is then used to simulate models of signaling networks in time-dependent geometries.

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MS75

A Forcing Method for Simulations of Chemical Transport in Blood Flow

The activated platelets in blood flow play a very important roles in blood clotting since they are at the central stage of the processes of aggregation and coagulation. To study the effect of chemical reactions on the surface of platelets for clotting, we use direct forcing formulation to treat the irregular and moving surfaces with Cartesian grid discretization of the computational domain. Both implicit and explicit form of the method will be showed for our problem.

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MS76

Nonnegative Polynomials and Sums of Squares

Sums of Squares (SOS) relaxations are often used as a substitute for testing whether a polynomial is non-negative. Testing whether a polynomial is SOS is a Semi-definite Programming problem and thus computationally tractable. We use techniques from convex geometry to study the relationship between sums of squares and non-negative polynomials. We will present results about the boundary structure and quantitative relationship between SOS and nonnegative polynomials, which allow us to understand the quality of SOS relaxations.

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MS76

Discriminants and Nonnegative Polynomials

For a semialgebraic set K in $\mathbf{R}^n$, let $P_d(K) = \{f \in \mathbf{R}[x]_{\leq d} : f(u) \geq 0 \, \forall u \in K\}$ be the cone of polynomials in $x \in \mathbf{R}^n$ of degrees at most d that are nonnegative on K. This paper studies the geometry of its boundary $P_d(K)$. When $K = \mathbf{R}^n$ and d is even, we show that its boundary $P_d(K)$ lies on the irreducible hypersurface defined by the discriminant $\Delta(f)$ of f. When $K = \{x \in \mathbf{R}^n : g_1(x) = \cdots = g_m(x) = 0\}$ is a real algebraic variety, we show that $P_d(K)$ lies on the hypersurface defined by the discriminant $\Delta(f, g_1, \ldots, g_m)$ of $f, g_1, \ldots, g_m$. When K is a general semialgebraic set, we show that $P_d(K)$ lies on a union of hypersurfaces defined by the discriminantal equations. Explicit formulae for the degrees of these hypersurfaces and discriminants are given. We also prove that typically $P_d(K)$ does not have a barrier of type $-\log \varphi(f)$ when $\varphi(f)$ is required to be a polynomial, but such a barrier exits if $\varphi(f)$ is allowed to be semialgebraic. Some illustrating examples are shown.

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MS76

Conic Representations for Positive Polynomials on

Equality-constraint Domains

We establish a simple connection between the set of polynomials that are non-negative on a given domain and the set of polynomials that are non-negative on the intersection of the same domain and the zero of a given polynomial. This connection has interesting algorithmic implications. For instance, it readily yields a succinct derivation of a copositive programming formulation for quadratically constrained quadratic programs.

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MS76
The Convex Hull of a Parametrized Curve

Understanding and computing the facial structure of the convex hull of a curve is generally a difficult problem. It becomes more tractable when the curve is parametrized by polynomials. We describe a general method for computing the boundaries of convex hulls of parametrized curves or segments of such curves. We'll give qualitative results in special cases, and we present many examples and pictures. Applications to spectrahedra, discrete geometry, and statistics will also be discussed.

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MS77
Open Discussion Moderated by:

Abstract unavailable at time of publication.

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MS77
Undergraduate and Graduate Training at the Rensselaer Polytechnic Institute

One of the challenges facing any applied mathematics program is to have students develop a strong mathematical foundation as well as an understanding of the relevant application areas. Our current approach includes close integration with researchers from multiple application disciplines, which includes lab work, involvement of our students in significant mentoring and leadership roles, and post-graduation involvement with our current students. This talk will review what we have done.

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MS77
Undergraduate Research Experiences in Computational Mathematics

I will describe several initiatives being undertaken at Arizona State University. (1) Undergraduate research experiences under the auspices of the NSF Computational Science Training Program for Undergraduates in the Mathematical Sciences; (2) the Computational Mathematical Sciences degree program; (3) curriculum development ideas at the advanced undergraduate level.

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MS77
Undergraduate CSE Programs in the U.S.

This talk will discuss the current state of Computaitonal Science programs in the US (and abroad) with reference to the updated SIAM Undergraduate CSE report. The new SIAM Undergraduate Research Online publication will also be presented as a suitable outlet for publishing quality undergraduate research in applied and computational mathematics.

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MS78
Channel Flow Simulations of a Microstructural Model for Wormlike Micellar Solutions ('Living Polymers')

The two-species VCM model is designed to capture the flow behavior of concentrated wormlike micellar solutions. The constitutive equations, which include scission and reforming (and viscoelastic relaxation) along with conservation of mass and momentum, form a coupled nonlinear system of partial differential equations. Simulations of the model in a pressure-driven channel flow, using an adaptive spectral collocation method, show that the velocity profile exhibits a plug-like (shearbanding) flow. Stability of the steady-state solutions is examined.

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MS78

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MS78

Kinetic-molecular Interaction Computation of Long-chain Polymer

Abstract unavailable at time of publication.

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MS78

A New Phase-Field Model for Incompressible Two-Phase Flows with Large Density Ratios

We present a new phase-field model for the incompressible two-phase flows with variable density which admits an energy law. We also construct weakly coupled time discretization schemes that are energy stable. Efficient numerical implementations of these schemes are also presented. The model and the corresponding numerical schemes are particularly suited for incompressible flows with large density ratios. Ample numerical experiments are carried out to validate the correctness of these schemes and their accuracy.

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MS79

Robust Principal Component Analysis?

This is about a curious phenomenon. Suppose we have a data matrix, which is the superposition of a low-rank component and a sparse component. Can we recover each component individually? We show that under mild conditions, it is possible to recover both the low-rank and the sparse components exactly by solving a very convenient convex program. This suggests the possibility of a principled approach to robust principal component analysis since our methodology and results assert that one can recover the principal components of a data matrix even though a positive fraction of its entries are arbitrarily corrupted. We present applications in the area of video surveillance, where our methodology allows for the detection of objects in a cluttered background.

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MS79

Mathematical Sensing , Dennis Healy's Vision

Throughout Healy's work before and during his Darpa years, we see sensing with coded waveforms as a tool for conversion of physical analog inputs into information. We will describe his visionary approaches to signal processing on the hardware , designed to achieve both efficiency in resources and higher information ratios , these include coded methodologies both passive and active for signal acquisition and processing.

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MS79

Deconvolution using Geometrically-based Representations

We propose deconvolution techniques based on transforming the data into geometrically-based representations such as the curvelet and shearlet representations. The representation implementations are designed to handle any assumed boundary conditions for the associated matrix inversion problem. Unique to these approaches is the ability to adaptively solve matrix inversion problems to estimate the coefficients of the representations by taking advantage of the different conditioning of the problems.

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MS79

Recent Advances in Computational Electromagnetics for Metamaterials

Metamaterial design will require rapid forward modeling of Maxwell's equations in complex microstructured materials. We will describe a new fast solver for this purpose that combines multiple scattering theory, high-order accurate integral equation discretizations and fast multipole acceleration.

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MS80

A Machine Learning Approach to Intrusion Detec-

tion for High Performance Computing

Abstract not available at time of publication.

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MS80

Compressively Sensed Complex Networks

We present a method, based on compressive sensing, to construct lossy compressions of complex networks. The method is based on the assumption that the adjacency matrix of the undirected complex graph can be represented compactly in some wavelet basis. We sample the adjacency matrix and reconstruct the original graph using a Staggered Orthogonal Matching Pursuit algorithm. We explore whether the compressed form of the graph can be used for comparison purposes.

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MS80

Cyber-Physical Trade-offs for Distributed Detection Networks

We consider a mathematical formulation of a generic detection problem using a network of sensors that measure intensity levels due to a source, whose intensity decays away from the source possibly in discrete jumps, and sensor measurements are random due to the nature of source and background. Under very general smooth and non-smooth conditions on source intensity functions and measurement distributions, we mathematically prove that better detection probability, compared to a single or co-located sensors, at any given false alarm probability can be achieved by: (i) spreading out sensors across the network, and (ii) utilizing measurements at the fusion center.

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MS80

Scalable, Parallel Stochastic Decomposition Algorithms for Risk Mitigation in Critical Infrastructure Applications

Abstract not available at time of publication.

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MS81

A Polynomial Time Algorithm for Optimizing over N-fold 4-block Decomposable Integer Programs

In this talk we generalize N-fold integer programs and two-stage integer programs with N scenarios to N-fold 4-block decomposable integer programs. We show that for fixed blocks but variable N, these integer programs are polynomial-time solvable for any linear objective. Moreover, we present a polynomial-time computable optimality certificate for the case of fixed blocks, variable N and any convex separable objective function. We conclude with two sample applications.

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MS81

On Algorithms Based on Cutting Plane Trees for General Mixed-integer Linear Programs

Recently, we gave a finite disjunctive programming procedure to obtain the solution of general mixed-integer linear programs with bounded integer variables, which we refer to as the *cutting plane tree (CPT) algorithm* (Chen et al, 2009). In this talk, we propose decomposition schemes to solve the cut generation problem arising in CPT effectively. We summarize our computational experience with the proposed algorithms.

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MS81

Local Search vs. LP for Matroid Matching

We consider the classical *matroid matching* problem. Unweighted matroid matching for linear matroids was solved by Lovász, and the problem is known to be intractable for general matroids. We present a PTAS for unweighted matroid matching for general matroids. In contrast, we show that natural LP relaxations that have been studied have an $\Omega(n)$ integrality gap and moreover, $\Omega(n)$ rounds of the Sherali-Adams hierarchy are necessary to bring the gap down to a constant. More generally, for any fixed $k \geq 2$ and $\epsilon > 0$, we obtain a $(k/2 + \epsilon)$-approximation for matroid matching in k-uniform hypergraphs, also known as the matroid k-parity problem. As a consequence, we

obtain a $(k/2+\epsilon)$-approximation for the problem of finding the maximum-cardinality set in the intersection of k matroids. We also design a 3/2-approximation for the weighted version of a known special case of matroid matching, the *matchoid problem*.

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MS81

Solving Symmetric Integer Programs

We will discuss mechanisms for dealing with integer programs that contain a great deal of symmetry. The methods use information encoded in the symmetry group of the integer program to guide the branching decision and prune nodes of the search tree. Computational results will demonstrate the great improvements in solution time obtainable when symmetry is exploited.

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MS82

Phase Field Methods for Strongly Anisotropic Systems

We study the influence of surface and strain energies on heteroepitaxial thin-film growth. We propose an alternate way of simulating anisotropy for the surface energy by using the higher order terms in the free energy. To the second order, the system only have isotropic properties. We can produce different anisotropy by adding higher order terms to the energy. By choosing the right parameters, we can study the behavior SiGe/Si thin film. This type of extended Cahn-Hilliard model has been previously studied to the 4th order, but to our knowledge no one has ever implemented all the terms in this system. One advantage of this energy is that it has the intrinsic regularization. We present numerical results using an adaptive, nonlinear multigrid finite-difference method.

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MS82

C^0 Penalty Methods for the Fully Nonlinear Monge-Ampere Equation

In this talk, we develop and analyze C^0 penalty methods for the fully nonlinear Monge-Ampere equation $\det(D^2u) = f$ in two dimensions. The key idea in designing our methods is to build discretizations such that the resulting discrete linearizations are symmetric, stable, and consistent with the continuous linearization. We are then able to show the well-posedness of the penalty method as well as quasi-optimal error estimates. Finally, we present some numerical experiments which support the theoretical results and discuss extensions to the three dimensional case as well as more general Monge-Ampere type equations.

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MS82

Convergent and Efficient Numerical Schemes for the Elliptic Monge Ampere Equation even in the Singular Case

The Monge-Ampere equation is challenging to solve numerically for the following reasons: 1. Singularites: If the source function f is not strictly positive, then solutions need twice differentiable. Weak (geometric) solutions allow even for f to be Dirac measure, which leads to solutions with corners. 2. The convexity constraint: the solution must be convex in order for the equation to be elliptic. Without the convexity constraint, this equation does not have a unique solution. In the singular case, many things break down: regularity, uniqueness, ellipticity of the equation. Correspondingly, from a numerical point of view, most solutions methods which rely on ellipticity become slow near singular solutions. In this talk we present and study the performance of three methods. The baseline method is provably convergent to the viscosity solution of the equation. For better performance, we study two other methods. The first method, which is simply the natural finite difference discretization of the equation, is more accurate, and the time to solve is independent of the regularity of the equation. The second method is faster in the non-singular case, but becomes very slow in the singular case. It also provided a model for generic methods which involve the solution of linear elliptic systems.

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MS82

Unconditional Stable Numerical Schemes for Phase Field Crystal (PFC) Equations

Highly efficient, unconditionally energy stable and uniquely solvable finite difference schemes for the Phase Field Crystal (PFC) equation, a nonlinear sixth order parabolic equation, are presented in the talk. A convex splitting of the corresponding physical energy is utilized. As a result, a combination of an implicit treatment for the convex part and an explicit treatment for the concave part leads to a numerical scheme with a non-increasing energy. Both the first and second order splittings in time, both the centered difference and the fourth order long stencil difference spatial approximations, are analyzed and proven to be unconditionally stable. In turn, a local in time numerical convergence can be derived. These ideas can be applied to other models of gradient systems, such as Cahn-Hilliard equations, a modified PFC model, epitaxial thin film growth models, etc. Some numerical simulation results are also presented in the talk.

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MS83

Data-free Inference of the Joint Distribution of Uncertain Model Parameters

While the correlation structure in the joint distribution of model parameters is critical to uncertainty analysis of the model, very often studies in the literature only report nominal values (and usually confidence intervals) for parameters inferred from data, but no details on the correlation or full joint distribution of these parameters. We demonstrate, using a Bayesian inference procedure, how to construct a posterior density for the parameters exhibiting self-consistent correlations, in the absence of data.

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MS83

Uncertainty Quantification in Inverse Problems for Subsurface Flows

In this talk, I will discuss uncertainty quantification in inverse problems with applications to subsurface flows. The inverse problem is set in Bayesian framework. The posterior probability distribution is complicated and involves solving systems of very large nonlinear PDEs. In this talk, I will focus on identifying permeability features such as facies and distribution within facies given integrated response, such as cumulative oil production. I will discuss sparse representations for the prior and efficient sampling techniques using multiscale models and hybrid techniques. This is a joint work with Anirban Mondal, Jia Wei, Bani Mallick and A. Datta-Gupta.

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MS83

Reducing Uncertainty in Inverse Problems by Design

Inverse problems are inertially ill posed and therefore no unique solution exists to the data fitting problem. One can use the wealth of regularization methods in order to obtain a unique solution. The question arise, how can we get better solutions to the problem? We shoe that the answer to this question can be tackled by analyzing the uncertainty in the problem. Both Bayesian and Frequentist approaches can be used. We show that while the statistical interpretation of each approach is different they lead to a rather similar mathematical treatment. We then discuss the solution of the design problem and show that better solutions can be obtained by using appropriate design

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MS83

The Effects of Data Assimilation on Uncertainty Propagation

The performance of popular uncertainty propagation schemes, including Monte Carlo methods, polynomial chaos, stochastic collocation, and sensitivity based methods are analyzed and assessed in a setting that is downstream of data assimilation. We devise a test problem where the source of uncertainty is generated by a process that is blinded from the uncertainty quantification process. Standard statistical method is performed to quantify the source of uncertainty, which is then propagated using various methods to the output quantity of interest. The methods for propagating uncertainty is assessed by comparing againt the true distribution of the quantity of interest, computed with knowledge of the process generating the source of uncertainty.

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MS84

Numerical Approximations of Stochastic Elliptic Models

The stochastic elliptic Model (I): $-\nabla\cdot(a(\mathbf{x},\omega)\nabla\mathbf{u}(\mathbf{x},\omega)) = \mathbf{f}(\mathbf{x})$ is widely used in engineering applications, where $a(\mathbf{x},\omega)$ is a positive random process, such as log-normal process. Another stochastic elliptic Model (II): $-\nabla\cdot(a(\mathbf{x},\omega)\diamond\nabla\mathbf{u}(\mathbf{x},\omega)) = \mathbf{f}(\mathbf{x})$ has also been widely studied, but mainly from the mathematical point of view, where $\diamond$ indicates the Wick product. We will show that Models (I) and (II) are in general not comparable. We then present a new stochastic elliptic model, which is also based on the Wick product, to establish the comparability with Model (I). Numerical results will be shown and related numerical issues will be discussed.

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MS84

Scattering of Shock Waves by Random Roughness:

Effects of Correlation Length

The oblique shock problem is a fundamental problem in high-speed aerodynamics and has been studied extensively. Instead of assuming smoothness, we take into account random roughness on the wedge surface to investigate the pressure distribution on the wedge. The roughness (of length d) starting at the wedge apex is modeled as stochastic process with zero mean and correlation length A. Both multi-element probabilistic collocation method (ME-PCM) on sparse grid and analysis of variance method (ANOVA) are employed to solve the stochastic Euler equations while a WENO scheme is used to discretize the equations in two spatial dimensions. The results by different methods are compared with the analytical solution obtained by the second-order stochastic perturbation analysis for small roughness height. We present the effects of different roughness length as well as different correlation length on the lift and drag forces on the wedge beyond the rough region. We also compare the accuracy and computational complexity of ME-PCM and ANOVA for different number of random dimensions in the representation of the random roughness.

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MS85

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS85

Modeling the Effect of an Enzymatic Inhibitor on Amyloid Beta Dynamics: The Role of Amyloid Clearance

Abstract not available at time of publication.

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MS85

An Analytic, Time-Dependent Model of a Product Development Pipeline

Abstract not available at time of publication.

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MS86

Ion Concentration Dynamics: a Novel Mechanism for Bursting and Seizing

We develop a conductance-based model neuron that includes intra- and extra-cellular ion concentration dynamics. We further formulate a reduction of this model to identify the bifurcation structure. Using these models, we describe a novel mechanism for bursting and seizing that results in behavior that is strikingly similar to that seen in experiments.

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MS86

Estimating the Directed Information to Infer Causal Relationships in Ensemble Neural Spike Train Recordings

Neuroscientists now often record many brain signals simultaneously. This provides potential to understand dynamic, complex, causal relationships in the brain. Here, we present a probably-good technique to estimate the directed information – an information-theoretic measure of causality philosophically wed to Granger causality. This is tested synthetically and correctly identifies all pairwise relationships. In ensemble M1 spike train recordings of an awake monkey, it identifies relationships consistent with wave propagation of simultaneously recorded local field potentials.

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MS86

Serotonin Chemistry and Neural Firing Patterns

Serotonin is a neurotransmitter that is thought to play an important role in mood, in eating behavior, in aggression and risk-taking, and in obsessive-compulsive disorder. A mathematical model for serotonin synthesis, release, and reuptake, is being used to understand the connections between serotonin metabolism and neural firing patterns. One goal of the project is to understand the mechanisms of action of selective serotonin uptake inhibitors. These mechanisms remain elusive despite years of experimental research.

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MS87

Multidimensional HLLE Riemann Solver; Applica-

tion to Euler and Magnetohydrodynamic Flows

In this work we present a general strategy for constructing multidimensional HLLE Riemann solvers. This is accomplished by introducing a constant resolved state between the states being considered, which introduces sufficient dissipation for systems of conservation laws. Closed form expressions for the resolved fluxes are also provided to facilitate numerical implementation. The Riemann solver is proved to be positively conservative for the density variable; the positivity of the pressure variable has been demonstrated for Euler flows when the divergence in the fluid velocities is suitably restricted so as to prevent the formation of cavitation in the flow. We also focus on the construction of multidimensionally upwinded electric fields for divergence-free magnetohydrodynamical (MHD) flows.

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MS87

Fast and Accurate Simulations of Proto-Planet Migration in Disks

In this talk, we present a fast and accurate numerical method for simulations of interaction between the protoplanetary disk and embedded proto-planets. Our hydro algorithm is at least an order of magnitude faster than other standard solvers. Our self-gravity solver costs less than 10% of the total computation cost. An embedded Lagrangian adaptive mesh refinement speeds up our computation by another order of magnitude.

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MS87

Hierarchical Reconstruction With Only Quadratic Remainder For Computing Non-smooth Solutions

In this talk I will briefly introduce the hierachical reconstruction (HR) useful for discontinuous Galerkin method (DG), central DG, central and finite volume schemes on regular or irregular meshes. In particular, A recently developed technique allows the use of only quadratic remainder in HR without hurting formal order of accuracy, which further improves the quality of numerical solutions for the 4th and 5th order cases.

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MS87

Simulations of Complex Flows using a Front Tracking Method

Numerical methods for multiphase flows have now made it possible to study in considerable detail the flow of hundreds of bubbles, drops, and solid particles. For more complex flows, such as those including phase change, mass transfer and chemical reactions, it is necessary to solve for additional physics that introduces new length and time-scales. Here, we discuss the extension of a front-tracking method for flows with sharp interfaces to deal with various complex flows.

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MS88

A Prototyping Effort in Developing an Engineering-Scale Nuclear Fuel Performance Code

Nuclear fuel undergoes substantial changes throughout nominal and transient operation as uranium fissions into new isotopes and the materials change due to macro- and micro-structural and chemical changes. This complex problem has historically leveraged one-dimensional approximations with empirical data for well- characterized fuels. This talk will explore the numerical and computational challenges associated with the development of a prototype code, AMP, which will be used to evaluate the physics-based requirements of a future predictive code.

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MS88

Overview of the Nuclear Energy Advanced Modeling and Simulation Waste Forms Integrated Performance and Safety Codes Program

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Forms (WF) Integrated Performance and Safety Codes (IPSC) is a new, long-term program responsible for providing an integrated suite of Thermal, Hydrological, Chemical, and Mechanical (THCM) computational modeling and simulation capabilities for predicting the performance of nuclear waste forms within storage or disposal repository environments. These capabilities will be used for predictive simulation-based, risk-informed decision making about managing future US nuclear waste.

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MS88

On Computational Frameworks for Multi-Physics Nuclear Reactor Simulation

Assembling a multi-physics reactor core simulation code requires a computational framework which can handle both legacy and more recent physics modeling components. These simulations must support execution at both ends of the performance spectrum, to allow both high-fidelity simulations (for the purpose of validation), and faster-running simulations informed by those higher-fidelity models, for use in design studies. In this talk we will describe the SHARP framework, which is being designed to meet these requirements.

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MS88

Phase Field Simulations of Irradiation-Induced Microstructure Evolution

The evolution of irradiation-induced defects such as voids and fission gas bubbles in nuclear fuel and structural alloys is critically important to the performance of fission reactors. Here, defect evolution in irradiated microstructure is modeled using a phase-field technique solved with a parallel finite element method. Multiple point defect species are randomly generated in space and time to represent collision cascade events and the effect of grain boundaries as well as stress gradients are also considered.

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MS89

A Hybridizable Discontinuous Galerkin Method for Steady-state Convection-diffusion-reaction Problems

We introduce a hybridizable discontinuous Galerkin method for steady-state convection-diffusion-reaction problems. The method is hybridizable, which renders it efficiently implementable. When the method uses polynomial approximations of the same degree for both the total flux and the scalar variable, optimal convergence properties are obtained for both variables; Moreover, the method exhibits superconvergence properties of the approximation to the scalar variable; this allows us to postprocess the approximation in an element-by-element fashion to obtain another approximation to the scalar variable which converges faster than the original one.

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MS89

A Two-grid Discontinuous Galerkin Method for Quasi Linear Elliptic Problems

We propose a two-grid discretization technique for the SIPG method for a class of quasi-linear elliptic problems. With the proposed technique, solving a quasi-linear elliptic problem on the fine space is reduced into solving a linear problem on the fine space and solving the quasi-linear elliptic problem on a much coarser space. A convergence estimate is derived to justify the efficiency of the proposed algorithm.

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MS89

A New Mixed Method for the Reissner-Mindlin Plate Model

The Reissner-Mindlin plate problem is written as a system of first order equations and all the resulting variables are approximated. A hybrid form of the method is presented which allows one to eliminate all the variables locally and have a final system only involving the Lagrange multipliers which approximate the transverse displacement and rotation at the edges of the triangulation. Optimal estimates independent of the plate thickness are proved for the transverse displacement, rotation and bending moment. A postprocessing technique is provided for the displacement variable and we show numerically that it converges faster than the original approximation. This work is in collaboration with Edwin M. Behrens.

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MS89

Higher Order Nonconforming Finite Elements for $H(curl) \cap H(div)$

Many problems in electromagnetics can be posed on subspaces of $H(curl) \cap H(div)$. However finite element subspaces of $(curl) \cap H(div)$ are necessarily subspaces of H^1 and therefore not appropriate for electromagnetic problems on nonconvex domains. On the other hand there is a natural interpolation operator from $H(curl) \cap H(div)$ into the well-known weakly continuous (vector) P1 element, which makes this nonconforming element useful for problems posed on $H(curl) \cap H(div)$ and general domains. In this talk we will discuss higher order nonconforming (vector) elements that have similar properties.

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MS90

Multi-Scale Methods for Simulating Turbulent At-

omization

Atomization involves processes on scales spanning several orders of magnitude. We will discuss numerical methods to address this multi-scale nature. These include the use of multiple concurrent meshes to resolve processes occurring on different scales, like turbulent flow structures, thermal boundary layers near the phase interface, and topology change events. In addition we will discuss a hybrid multiscale Eulerian/Lagrangian technique to deal with the vast number of spray droplets generated in atomization.

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MS90

Multiphase Flows in Complex Geometries: A Diffuse Domain Approach

We present a new method for simulating two-phase flows in complex geometries, taking into account contact lines separating immiscible incompressible components. We combine the diffuse domain method for solving PDEs in complex geometries with the diffuse-interface (phase-field) method for simulating multiphase flows. In this approach, the complex geometry is described implicitly by introducing a new phase-field variable, which is a smooth approximation of the characteristic function of the complex domain. The fluid and component concentration equations are reformulated and solved in larger regular domain with the boundary conditions being implicitly modeled using source terms. The method is straightforward to implement using standard software packages; we use adaptive finite elements here. We present numerical examples demonstrating the effectiveness of the algorithm. We simulate multiphase flow in a driven cavity on an extended domain and find very good agreement with results obtained by solving the equations and boundary conditions in the original domain. We then consider successively more complex geometries and simulate a droplet sliding down a rippled ramp in 2D and 3D, a droplet flowing through a Y-junction in a microfluidic network and finally chaotic mixing in a droplet flowing through a winding, serpentine channel. The latter example actually incorporates two different diffuse domains: one describes the evolving droplet where mixing occurs while the other describes the channel. This is joint work with Sebastian Aland and Axel Voigt.

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MS90

A Pointwise Second-Order AccurateVolume-of-Fluid Interface Reconstruction Algorithm

I will describe a volume-of-fluid interface reconstruction algorithm that is second-order accurate pointwise, provided the curve $\mathbf{z}(x(s), y(s))$ is two-times continuously differentiable and the (non-dimensional) grid size h satisfies $\kappa_{max} \leq \min\{C_h h^{-1}, (\sqrt{h})^{-1}\}$ locally, where κ_{max} is the (non-dimensional) local maximum of the curvature $\mathbf{z}$. I will present examples of computations and an outline of a proof that this method is second-order accurate in the max norm.

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MS90

Field-induced Motion of a Ferrofluid Droplet in a Viscous Medium

The effect of applied magnetic fields on the deformation of a biocompatible hydrophobic ferrofluid drop suspended in a viscous medium is investigated numerically and compared with experimental data. At high magnetic fields, experimental drop shapes deviate from numerical results when a constant surface tension value is used. One hypothesis for the difference is the dependence of interfacial tension on the magnetic field in the experimental data. This idea is investigated computationally.

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MS91

Dynamic Moduli of Nematic Liquid Crystal Polymers with Parallel Anchoring Conditions

We apply anchoring conditions to a nematic liquid crystal polymer system so that the major director lies parallel to the plates of a shear cell and then apply a small amplitude shear flow at an arbitrary angle to the direction of the anchoring. We use a Doi-Marrucci-Greco tensor model with one dimensional heterogeneity to predict the dynamic moduli. For anchoring that lies in the flow-flow gradient plane, the system effectively recovers Leslie-Ericksen theory. If logrolling anchoring, the solution is also analytically solvable. For the oblique angles in between in-plane and logrolling, we solve the system numerically. The viscosity is smaller for logrolling anchoring than in-plane, and logrolling thins above a critical frequency, unlike in-plane anchoring. The in-plane storage modulus is slightly larger than logrolling for low frequencies. However, for higher frequencies, logrolling can be two-to-three orders of magnitude larger than in-plane.

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MS91

Stability of Active Suspensions

We investigate the linearized structure of a recently derived kinetic model describing suspensions of active particles near a state of uniformity and isotropy. We show that system instability can arise only from the dynamics of the first azimuthal mode in swimmer orientation, and that at small-scales the system is controlled independently of the nature of the suspension. A prediction about the onset of the instability is made.

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MS91

An Integrative Model of Spermatozoa Motility

Calcium (Ca^{2+}) dynamics in mammalian sperm are directly linked to motility. These dynamics depend on diffusion, nonlinear fluxes, Ca^{2+} channels specific to the sperm flagellum, and other signaling molecules. The goal of this work is to couple Ca^{2+} dynamics to a mechanical model of a motile sperm within a viscous, incompressible fluid. We will present recent progress on elements of this integrative model.

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MS91

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MS92

Efficient Methods for Random Field Approximation with Application to Nonlinear Schr?odinger Equation

Either due to the randomness in nature or the insufficiency of knowledge, most physical or engineering systems involve uncertainty to a certain degree. To gain a better understanding of the intrinsic dynamics, such uncertainty should be modeled and analyzed. Bose-Einstein condensate (BEC) with disorder is such an example. In physical experiments, the disorder (or random potential) has been generated through optical speckle patterns, and stable soliton waves were observed when the disorder has appropriate strength. But the complete dynamics of the solution is still largely unknown. This prototype problem can be modeled by the nonlinear Schrödinger equation (NLSE) with a random potential (also called the *Gross-Pitaevskii* equation), which governs the evolution of the mean-field wave function in BECs. We study the formation and evolution of the soliton waves in the 1D and 2D NLSEs with a random potential.

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MS92

A Local Vorticity Boundary Condition Spectral Collocation Method for 2D Incompressible Fluids

A simple spectral collocation method for viscous incompressible flow in a bounded 2D domain is presented for the vorticity-stream function formulation of the incompressible Navier-Stokes equations, along with its extension to the Boussinesq system. The no-slip boundary condition for velocity is converted into a local boundary formula for the vorticity, which when used in conjunction with an explicit time stepping scheme allows decoupling the computation of the vorticity and stream function time updates. Numerical results are presented for the singular lid-driven caivity problem, a benchmark differentially heated cavity problem, and a Rayleigh-Bernard convection problem for Rayleigh number up to 10^{10}, demonstrating the efficiency of the method, and in particular that it is well suited for high Reynolds or high Rayleigh number regime simulations.

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MS92

Numerical Simulation of Cahn-Hilliard-Hele-Shaw Equations

Unconditionally energy stable and solvable schemes for the Cahn-Hilliard-Hele-Shaw (CHHS) equation are presented

in the talk. This equation arises in models for spinodal decomposition of a binary fluid in a Hele-Shaw cell, tumor growth and cell sorting, and two phase flows in porous media. A convex splitting technique for this specialized conserved gradient flow is utilized, which gives a non-increasing energy. Some numerical simulation results are also presented in the talk.

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MS92

An Unconditionally Stable Second-Order Scheme for the Slope Selection Equation and Related Epitaxial Thin Film Models

In this talk I describe a second-order convex splitting scheme for the Slope Selection equation, which is a model thin film roughening and subsequent coarsening. Like the first-order convex splitting scheme that we introduced in an earlier work, the scheme is unconditional energy-stable (and norm stable) and unconditionally uniquely solvable. I prove that the (fully discrete) scheme results as the gradient of a strictly convex functional, and hence gradient-based solvers, e.g., Newton's method, are globally convergent. In the talk I discuss issues concerning practical and efficient solution of the scheme using nonlinear multigrid and nonlinear conjugate gradient methods. This work is joint with Cheng Wang (UMass) and Xiaoming Wang (FSU).

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MS93

A Multi-explicit Spectral Deferred Correction Method Applied to Regularized Stokeslets

In this discussion, regularized Stokeslets are used to model immersed elastic objects with stiff spring forces. In certain scenarios, the fluid velocity can be decomposed to isolate stiff terms. The multi-explicit spectral deferred correction method utilizes such a decomposition and integrates stiff velocity components with a small time step while treating non-stiff components with a larger time step. This eliminates unnecessary expensive calculations while still treating the system explicitly in a stable, efficient manner.

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MS93

Integral Deferred Correction and High Order Splitting Method for PDEs

Integral Deferred Correction (IDC) belongs to the general family Defect Correction (DC)algorithms. IDC differs from traditional DC in that the integral of the residual appears in the error equation rather than the derivative of the residual. In this work, we investigate several formulations of IDC in order to generate high order split methods for a range of PDEs. The eventual goal is to develop efficient methods for high order phase field models on GPUs.

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MS93

Combining a Multi-grid Approach with Deferred Correction Methods

In a deferred correction method, a standard numerical method is used to first compute a provisional solution at a number of intermediate points in a integration interval. Then an equation for the error in the approximation is constructed and solved iteratively using a low-order method to generate increasingly accurate approximations. By combining a multi-grid approach with the deferred correction methods, we obtained a class of methods that are highly efficient in computing high-order approximations for multiscale partial differential equations.

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MS93

RIDC: Parallel High-order Time-stepping

RIDC (revisionist integral deferred correction) methods are a class of time integrators well-suited to parallel multicore computing. RIDC methods can achieve high-order accuracy in wall-clock time comparable to forward Euler. The methods use a predictor and multiple corrector steps. Each corrector is lagged by one time step; the predictor and each of the correctors can then be computed in parallel. This presentation introduces RIDC methods and demonstrates their effectiveness on some test problems.

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MS94

Mathematical Tools for Management of System Complexity

My conversations with Dennis always included issues in complexity, be it on tools for characterizing complexity of system design, its architecture or management of complexity in engineered systems. In this talk I will reflect on these topics within the context of dynamical systems theory and discuss various tools for taming complexity, many coming from the realm of harmonic analysis, but also utilizing graph theory and ergodic theory. I will also highlight discussions we had on architecture of microfluidic systems and our ideas on architecture of microengines.

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MS94

Moving Innovation Forward: The Biosensors Program at NIH

In 2000, the National Institute on Alcohol Abuse and Alcoholism (NIAAA), part of the National Institutes of Health (NIH), embarked on a small but innovative venture, modeled in part on DARPA. The first goal of the program was the development, in five years, of biosensors for alcohol consumption in humans. Dennis Healy was asked to head this effort, working with NIH staff in development of the program. Dennis didn't want merely to develop sensors, however. His idea was to push development and innovation a step further, by requiring each sensor to have a fully integrated data analysis system. In 2002, 5 unique biosensor system projects were funded. Two of these systems will be described, highlighting the integration of science, engineering, and mathematics in their design, as well as how these systems fit into Dennis' vision for biomedical applications of sensor technologies.

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MS94

Manifold Matching Classification: Joint Optimization of Fidelity and Commensurability

We consider the statistical pattern recognition task in which data is available in multiple disparate spaces, but no data belonging to the classes of interest is available in the space of interest. We consider fusion and inference from multiple disparate data sources via joint optimization of fidelity and commensurability.

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MS94

Dennis Healy's work at Dartmouth in Computational Harmonic Analysis

In this talk we survey Dennis Healy's tenure at Dartmouth and his significant contributions to applied and computational noncommutative Fourier analysis and wavelet analysis. In particular, his work on an FFT for the 2-sphere and his work in fast MRI.

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MS95

Cutting Planes and Maximal Lattice-free Convex Sets

This talk is based on joint work with Borozan, Basu, Conforti and Zambelli. We consider a model that arises in integer programming, and show that all irredundant inequalities are obtained from maximal lattice-free convex sets in an affine subspace. We also show that these sets are polyhedra. The latter result extends a theorem of Lovász characterizing maximal lattice-free convex sets in R^n.

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MS95

Some Relationships between Disjunctive Cuts and Cuts based on S-free Convex Sets

Pursuing a line of research proposed by Balas (2009), we establish exact correspondence between 2-branch disjunction and a strict subclass of S-free cuts for the two row constrained group relaxation (2RCGR). We propose a new class of nonsymmetric 2-branch disjunctive operation that can be used to obtain all the 2d S-free cuts for 2RCGP. We also study relationship of symmetric and nonsymmetric disjunctions applied to general mixed integer sets with cuts from its 2RCGRs.

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MS95

On Families of Split Cuts that can be Generated Efficiently

We study several heuristics to generate new families of split cuts, by considering integer linear combinations of the rows of the simplex tableau, and deriving the corresponding mixed-integer Gomory cuts. In particular, we propose several cut generation algorithms that share the following aims: reducing the number of nonzeroes, obtaining small coefficients, generating orthogonal cuts. We present a computational evaluation that shows the usefulness of these new cuts in a Branch-and-Cut framework.

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MS95

On the Rank of Cutting-plane Proof Systems

We introduce a natural abstraction of propositional proof systems that are based on cutting planes. This new class of proof systems includes well-known operators such as Gomory-Chvátal cuts, lift-and-project cuts, Sherali-Adams cuts, and Lovász-Schrijver matrix cuts. We show that whenever a specific cutting-plane based proof system has (maximal) rank n on a particular family of instances, then any cutting-plane proof system in our class has rank $\Omega(n/\log n)$ for that family. We also construct a new cutting-plane proof system that has worst-case rank $O(n/\log n)$ for any polytope without integral points, showing that the universal lower bound is essentially tight. Furthermore, we prove that whenever some cutting-plane proof system in our class has rank n, then the rank of any one of the known proof systems mentioned above is at least $n-1$. Finally, we provide a complete characterization of all polytopes without integral points in the n-dimensional 0/1-cube of maximal Gomory-Chvátal rank n.

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MS96

Nontraditional Tensor Decompositions and Applications

This presentation will discuss two tensor decompositions that are not as well known as PARAFAC (parallel factors) and Tucker, but have proven useful in informatics applications. Three-way DEDICOM (decomposition into directional components) is an algebraic model for the analysis of 3-way arrays with nonsymmetric slices. PARAFAC2 is a related model that is less constrained than PARAFAC and allows for different objects in one mode. Applications of both models to informatics problems will be shown.

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MS96

Small Tensor Rank is in RP

Hastad has shown that determining the rank of a 3-tensor is an NP-hard problem in general. Nevertheless Hastad's construction involves a $l \times m \times n$ tensor of rank strictly larger than $\max(l, m, n)$. We show that if we restrict ourselves to tensors of rank not more than $\max(l, m, n)$, then the rank of such tensors may be computed in randomized polynomial (RP) time. A consequence is that computing rank for this smaller class of tensors is unlikely to be in NP (unless of course P = NP). We will discuss a readily implementable algorithm.

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MS96

Incorporating Intervariable Geminals into Sums of Products

Representing a multivariate function as a sum of products of one-variable functions bypasses the curse of dimensionality. However, the wavefunction of a quantum-mechanical system has dependencies on the differences of pairs of variables, which makes such sums converge slowly. A representation with intervariable geminals times sums of products should allow faster convergence. This representation requires interesting algorithms, which can be represented as sequences of graphs.

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MS96

Matters of the Heart: Mathematical Modeling with Tensors

This talk focuses on the possible development, analysis and computer implementation of mathematical models of the cardiovascular system. Our goal is to automatically gauge the anatomic structure and the physiological response of the human cardiovascular system as healthy or diseased states. The mathematical analysis of these problems is complicated and the related numerical analysis difficult. Our goal encompasses the idea of representing data that have been extracted non-invasively as 3-dimensional tensors. This include fore mostly, echocardiograms, electrocardiograms and perhaps MRI's as these methods have minimal invasion to the patient and the resulting data can be viewed as a sequence of related images (matrices). Traditional numerical linear algebra is not enough in these data mining applications; a comprehensive set of numerical multilinear algebra tools will be required to spot patterns in n-way data. Tensor decompositions have proven to be successful in extracting the underlying structure in such datasets.

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MS97

Distributional Sensitivity Analysis for Factor Prioritization

Factor prioritization is the identification of factors causing the greatest reduction in output variance when subject to factor uncertainty reduction, and is an important aspect of the application of complex models for decision-making. We present a distributional sensitivity analysis for factor prioritization that assumes the portion of a particular factor's variance that can be reduced is a random variable. Our method is applied directly to the results of a global sensitivity analysis using acceptance/rejection sampling.

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MS97

Numerical Solutions of Optimal Control Problems Governed by Stochastic Partial Differential Equa-

tions

Abstract not available at time of publication.

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MS97

Distributional Sensitivity for Uncertainty Quantification

In this talk we present a novel technique that quantifies sensitivity in a model when epistemic uncertainty is present in the density function of random variables. This nonintrusive method is easily applicable to existing codes and can easily be implemented as a post-processing operation. Using generalized Polynomial Chaos, we show examples illustrating the effectiveness and efficiency of our approach.

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MS97

Stochastic Optimal Design of Complex Systems using Approximate Models

We advocate a simulation strategy that recasts the optimization problem as a sampling problem in the expanded space which apart from the random variables includes the design parameters. To that end we employ adaptive Sequential Monte Carlo (SMC) methods that scale well in high dimensions, are directly parallelizable and can identify multimodal densities. We propose a hierarchical strategy where approximate forward models can be rigorously incorporated in order to give accurate estimates at a reduced computational cost.

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MS98

Optimal Experimental Design in Biological Applications

Dynamical systems are the right tool to simulate and model biological systems. In biological disciplines the choice of the design of an experiment is most important to recover model parameters. The strong interplay between accuracy of the results and efficiency of experiment need to be considered carefully. We present the computational framework for ordinary differential equations, optimization, parameter estimation, and optimal experimental design and apply these methods to target the questions arising from the biology.

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MS98

Optimal Choice of Sample Times

Based on an abstract notion of sampling procedures involving probability measures on the sampling interval we present an algorithm for determining optimal sampling times in the given sampling interval. Fundamental for the approach is the fact that the set of probability measures on an interval is a metric space under the so called Prohorov metric. As optimality criterion one can take any continuous function of the Fisher information matrix corresponding to the chosen sampling times.

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MS98

Optimal Design for Imaging

Experimental design is an important topic for imaging science. It has broad applications in the areas of physics, biology and engineering. In this talk, we examine the Bayesian A and A_π optimal designs. Our methods have the capability to improve the image quality while maintaining low experimental cost. Several imaging experiments, such as super resolution will be presented. Moreover, we explore efficient methods for large scale design problems.

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MS98

Optimal Experimental Design in Geophysical Applications

In this talk we discuss the design of experiments for ill-posed problems that arise in biological applications. We show that the problem is cast is a nonlinear stochastic programming problem and suggest efficient methods for its solution. We then discuss biological applications and show the effectiveness of our approach.

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MS99

Compressed Sensing: How Sharp is the RIP?

The Restricted Isometry Property (RIP) has become a

widely used tool for the analysis of signal recovery algorithms used in compressed sensing. Through an asymmetric interpretation of the RIP and by developing the best known bounds on the RIP constants for matrices from the Gaussian ensemble, we are able to make quantitative statements regarding the theoretical guarantees for these algorithms. Moreover, we translate these results into the phase transition framework advocated by Donoho et al. which permits direct comparison across algorithms and to alternative methods of analysis.

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MS99

Overview of Rhase Transitions in Compressed Sensing

In my slot, I will try to address non-experts. I will prepare the stage for other speakers in this session by explaining the significance of phase transitions in compressed sensing as signifying 'undersampling theorems' that place useful limits on how much we can undersample, and surveying some of what is currently known and what remains to be studied.

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MS99

Various Thresholds for ℓ_1 Optimization in Compressed Sensing

Recent works of Candes, Romberg, and Tao, and Donoho theoretically analyzed the success of a polynomial ℓ_1 optimization algorithm in solving an under- determined system of linear equations. In a large dimensional and statistical context it was proved that if the number of equations (measurements in the compressed sensing terminology) in the system is proportional to the length of the unknown vector then there is a sparsity (number of non-zero elements of the unknown vector) also proportional to the length of the unknown vector such that ℓ_1 optimization succeeds in solving the system. In this talk, we discuss an alternative performance analysis of ℓ_1 optimization which allows for computing proportionality constants of recoverable sparsity that are comparable to the best currently known ones obtained by Donoho.

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MS99

The Balancedness Properties of Linear Subspaces with Applications in Compressive Sensing

In this talk, we investigate the ℓ_1 "balancedness" properties of linear subspaces in E^n, namely a small index set can not support too much ℓ_1 norm, and discuss the applications of these properties in compressive sensing. We will first give the definitions of weak,sectional and strong "balancedness" properties for linear subspaces and their applicaitons in sharply characterizing or bounding the performances of compressive sensing. Using tools from high dimensional integral geometry and geometric probability, we give a unified Grassmann Angle framework for analyzing these "balancedness" properties, and give sharp performance bounds for the "balancedness" that a linear subspace can achieve in various cases. We will further discuss the applications of this analytical framework in analyzing and designing powerful signal recovery algorithms such as weighted or iterative reweighted ℓ_1 minimization algorithms. This work concerns random projections of high dimensional polytopes and fundamental properties of linear subspaces, so it may be of independent mathematical interest. Recent progress on investigating the ℓ_p, $0 < p < 1$ "balancedness" property will also be discussed. This series of work is by collaboration with Babak Hassibi (Caltech), Amin Khajehnejad (Caltech), Salman Avestimehr (Cornell), Meng Wang (Cornell), and Kevin (Ao) Tang (Cornell).

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MS100

Investigating the Role of Dynamics in a Model Orexin Neuron's Response to Orexin and Dynorphin

Narcolepsy is associated with a loss of signaling in the orexin (hypocretin) system. Local interactions within the orexin neuron field are mediated by the neuropeptides orexin and dynorphin. These neuropeptides appear to be colocalized in orexin neurons and exert excitatory and inhibitory autoeffects, respectively. However, different rates of desensitization result in complex responses to orexin/dynorphin coapplication. In a Hodgkin-Huxley-type model orexin neuron, we investigate the role of both intrinsic and network dynamics in these responses.

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MS100

Multivariate Point Process Representations of Ensemble Neural Spiking Activity

Understanding how ensembles of neurons represent and transmit information in their joint spiking activity is a fundamental question in neuroscience. We develop a new simultaneous event multivariate point process model that can represent simultaneous occurrences of spike events at an arbitrarily small time resolution and use it to analyze ensemble spiking activity from rat thalamic neurons recorded in response to whisker stimulation. This new model has important implications for deciphering neuronal representations.

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MS100

Differential Contribution of Potassium Currents to Neuronal Excitability

The excitability of a neuron depends on the different inward and outward currents that flow across its membrane. Drosophila is used as a model system to examine the theoretical plausibility of existing hypotheses about the differential involvement of A-type currents in delaying spiking activity. The model is constructed using known macroscopic biophysical properties of voltage-dependent, slowly inactivating and fast inactivating A-type channels and constrained using electrophysiological data.

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MS100

A Minimal Biophysical Model of Phase Precession

Some pyramidal cells in the rodent hippocampus called place cells, fire at specific locations called place fields during spatial tasks. The spiking in place cells is also modulated by oscillations in the local field potential. As the rat moves through a place field, place cell firing occurs at progressively earlier phases of the oscillation within the theta band (7-12 Hz). A minimal biophysical model is used to study phase precession.

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MS101

Central Discontinuous Galerkin Methods for MHD Equations

In this talk, central discontinuous Galerkin (DG) methods will be presented for ideal MHD equations. Originally introduced for hyperbolic conservation laws and recently developed for Hamilton-Jacobi equations, central DG methods combine ideas in central schemes and DG methods. They avoid the use of Riemann solvers which are complicated and costly for MHD equations, while evolving two copies of approximating solutions on overlapping meshes.

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MS101

Compact Integration Factor Methods for Complex Domains and Adaptive Mesh Refinement

To reduce the cost of solving stiff reaction diffusion equations, we introduce a compact implicit integration factor (cIIF) method for efficient storage and calculation of exponential matrices associated with the diffusion operators. In addition, we present a method for integrating cIIF with adaptive mesh refinement (AMR) with large time steps by taking advantage of excellent stability condition for cIIF. An example of simulating a cell signaling system is given to show excellent performance.

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MS101

Eulerian Flow Solvers for Three Temperature Plasma Physics

We study a plasma physics model that includes electron heat conduction and energy exchange between electrons and ions. For simple shock flows, the model reduces to an autonomous system of ordinary differential equations that allows for a phase space analysis and semi-analytical solutions. 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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MS101

A Conservation Constrained Discontinuous Galerkin Method with Improved CFL Number for Conservation Laws

We present a new formulation of the RKDG method for conservation Laws, which requires the computed RKDG solution in a cell to satisfy additional conservation constraint in adjacent cells. This new formulation improves the CFL number over the original RKDG formulation without increasing the complexity comparing with the regular RKDG formulation. It also effectively improves the robustness of the DG scheme and improves the resolution of the numerical solutions in multi-dimensions.

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MS102

Simulations of Xe Redistribution in Uranium Dioxi

Abstract unavailable at time of publication.

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MS102

Numerical and Software Engineering Challenges in the NEAMS Waste Forms Sub-Program

Abstract unavailable at time of publication.

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MS102

Scalable Methods for the Neutron Transport Equation under Development at Argonne National Lab-

oratory

Abstract unavailable at time of publication.

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MS102
Controlling Defect Segregation in Uranium Dioxide

Abstract unavailable at time of publication.

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MS103
On FEM Approximations to the Navier-Stokes Equations with Scott-Vogelius Elements

Abstract unavailable at time of publication.

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MS103
A Strongly Conservative, Monolithic Finite Element Method for Stokes-Darcy Coupling

Divergence conforming finite elements have been applied successfully to the Stokes and Navier-Stokes problem, using discontinuous Galerkin techniques. On the other hand, these elements are natural for porous media flow modeled by Darcy's equations. In this presentation, we will show the opportunities offered by a uniform discretization with Raviart-Thomas elements for the free and the porous media flow. The stability of the method will be discussed and numerical examples will confirm the applicability of the new scheme.

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MS103
Penalty-factor-free Discontinuous Galerkin Methods for 2-dim Stokes Problems

We present two new finite element methods for two-dimensional Stokes problems. These numerical schemes are developed by relaxing the constraints of the classical Crouzeix-Raviart nonconforming P_1 finite elements. Penalty terms are introduced to compensate lack of continuity or divergence-free property. However, there is no need for choosing penalty parameters and the formulations are symmetric. These new methods are easy to implement and avoid solving saddle-point linear systems. Numerical experiments are presented to illustrate the proved optimal error estimates.

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MS103
A Posterior Error Estimate for Finite Element Methods for the Stokes Equations

We establish a posterior error analysis for finite element methods of the Stokes equations. This residual estimator can be applied to almost all the existing finite element methods including conforming, nonconforming and discontinuous finite elements.

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MS104
Adaptive Mesh Refinement Techniques for Free Boundary Problems

In this talk, I will describe a new paradigm for solving partial differential equations on Quadtree/Octree grids. In particular, I will describe the level-set technology and how to enforce implicitly boundary condition at a moving front. Examples will include single and two-phase flows as well as the solution of the Poisson-Bolztmann equations.

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MS104
Numerical Analysis of Non-extensible Interfaces in Incompressible Flow

Non-extensible but deformable interface in an incompressible flow, for example, shear flow, can be used to study the deformation of red blood cells in mathematical biology. The governing equations are incompressible Stokes or Navier-Stokes equations with an unknown surface tension that should be determined in a such way that the interface is incompressible along the tangential direction. Thus the problem is essential an inverse problem that is sensitive to perturbations. In the literature, often boundary integral methods are used for Stokes flows. Geometrically, the problem implies that both the area and the length of the cell should be preserved as the interface evolves. In this talk, we present the immersed interface method with some regularization technique for simulating such problems with both Stokes and Navier-Stokes equations. For Navier-Stokes equations, we propose a modified projection method so that the pressure jump condition corresponding to the unknown surface tension can be strictly enforced. In our numerical methods, the bending force can be also included. Numerical analysis are carried out with different Reynolds numbers, circularity, and the initial orientation of the cells.

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MS104

Stability Analysis of a Coflowing, Bended, Gas/liquid Jet Flow

A Numerical technique based on the pseudo-spectral method is presented for performing a linear spatial stability analysis for a bended co-flowing gas/liquid jet. The numerical method that will be presented is an extension of the method developed by Gordillo and Perez-Saborid (2005) for a non-bended co-flowing gas/liquid jet. The linear stability analysis of a bended liquid jet is applied to the problem of the break-up of a liquid jet in a cross-flow. Results of the linear stability analysis are compared against the results derived from directly computing solutions of the original two-phase Navier-Stokes equations.

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MS104

Multiscale Issues in DNS of Multiphase Flows

In DNS of multiphase flows it is frequently found that features much smaller than the "dominant' flow scales emerge. Those features consist of thin films, filaments, and drops, and usually the geometry is simple and inertia effects are relatively small for the local evolution. In isolation these features are therefore often well described by analytical models. Here we describe the use of thin film models as subgrid models in DNS of multiphase flows.

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MS105

Mapping Communication-Avoiding QR Decomposition to Various Architectures

The large and increasing costs of communication motivate redesigning algorithms to avoid communication whenever possible. Recent development of the "Communication-Avoiding QR" algorithm has been shown to minimize (in an asymptotic sense) the communication costs of computing the QR decomposition on either a sequential or parallel computer, yielding speedups over conventional algorithms in both theory and practice. In order to minimize communication, the algorithm must be mapped to the underlying architecture. In this talk we will discuss how this mapping is done for a sequential machine and a distributed-memory parallel machine, and we will discuss extensions of the algorithm to other interesting architectures.

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MS105

Numerical Policy Function on Auto-tuned Sparse Iterative Solver Xabclib

Conventional auto-tuning software focuses on optimization with execution speed. However, the requirement of auto-tuning depends on situation of software usage for end-users. In this presentation, we develop a new function of auto-tuning, named "Numerical Policy Function". The policy function optimizes execution speed, memory amount, and computational accuracy. A result of performance evaluation will be shown with one node of the T2K Open super computer (16 cores) for the Xabclib, which is an OpenMP parallelized numerical library with the policy function for sparse iterative solvers. The Xabclib is also implemented with OpenATLib, which is a library of APIs to establish common interface for auto-tuning functions.

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MS105

Redesign of Higher Level Matrix Algorithms for Multicore and Hybrid Architectures: A Case Study for Green's Function Calculation in Quantum Monte Carlo Simulation

The emerging multicore computing systems require significant modification to today's computational tools and technologies. A great deal of efforts have been focused on the redesign of essential matrix computations, such as matrix multiplication or the QR decomposition for optimal performance on multicore systems. However, by nature, not every matrix operation can be efficiently parallelized, for example, the QR decomposition with column pivoting, and explicit matrix inversion. The performance of these matrix operations is still lack behind and substantial slower on parallel environments. In this paper, we take an approach to re-design numerical algorithms for higher-level algorithm so that they only uses easily parallelizable linear algebra building blocks: matrix multiplication and QR decomposition', but not column pivoting and the explicit matrix inversion. Specifically, we will redesign the higher-level algorithms for communication avoidance in the application of quantum Monte Carlo simulation. A new algorithm, called structure orthogonal factorization (SOF), is proposed for parallelizing the Green's function calculations, it only uses easily parallelizable linear algebra building blocks and significantly reduces the communication cost. The new algorithm is as stable as the previous algorithm. The previous algorithm requires less flops but uses the QR decomposition with column pivoting, which is a communication intensive. Although the new algorithm uses a factor of 3 more flops than the previous algorithm, it is 16% faster on a quad-core system, and 2.5 times faster on a 1024-CPU hybrid systems.

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MS105

Automatic Tuning for Parallel 3-D FFTs

In this talk, an implementation of parallel 3-D fast Fourier transform (FFT) with automatic performance tuning method is presented. An blocking algorithm for parallel FFTs utilizes cache memory effectively. Since the optimal block size may depend on the problem size, we propose a method to determine the optimal block size that minimizes the number of cache misses. Performance results of parallel 3-D FFTs on clusters of multi-core processors are reported.

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MS106

Investigating a Convective Cloud Feedback Mechanism for Warm Climates using Simple and Complex Climate Models

Complex climate models have difficulty simulating the Arctic climate of ancient warm periods and diverge impressively in their forecast of future sea ice at high CO2. A convective cloud feedback has been proposed that might help resolve these issues. The strength of this feedback and CO2 at which it activates vary widely among the models. Here we use a hierarchy of climate models to investigate the factors that control the activation and strength of this feedback.

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MS106

Multiple Scales in Numerical Models of Ocean Circulation

The circulation of the ocean plays a major role in the global climate system. A fundamental property of this circulation is its very wide ranges of space and time scales. In keeping with the purposes of this minisymposium, this talk will include a general survey of how these ranges of scales can influence modelers' choices of time discretization, vertical coordinate, and physical parameterizations. I will also outline some of my own work on time splitting and time stepping and make some comments about spatial discretizations.

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MS106

Mathematical Issues in Data Assimilation of Data and Models in Climate Research

Climate data is remarkably sparse and poorly constrained, and models for climate are far from complete. How does one make meaningful forecasts? What are the challenges in this peculiar forecasting framework? What are the tools? I will frame these questions, provide a survey of key ideas, and show some of the work done by my group in nonlinear non-Gaussian data assimilation.

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MS106

Bifurcations, and their Implications, in a Simple Model of Arctic Sea Ice

Eisenman and Wettlaufer (PNAS 2009) proposed a simple ODE model for Arctic sea ice subjected to seasonally-varying solar forcing. We extend their box model to describe both polar and subpolar sea ice, and analyze the dynamics of the coupled system. Subpolar winter sea ice loss is abrupt and causes complete sea ice loss in the polar region as well. Summer sea ice loss does not show threshold behavior and progresses smoothly from south to north.

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MS107

Near Field Imaging of the Surface Displacement on An Infinite Ground Plane

This work is concerned the numerical study of the inverse diffraction problem for an unbounded obstacle. The obstacle is a ground plane with a local disturbance. A reconstruction scheme based on the integral equation method is proposed to image the surface displacement at near field. The method utilizes the evanescent waves effectively, which significantly improves the spatial resolution of the image. The on-going research project on this topic will also be highlighted.

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MS107

A New Approximations of Effective Hamiltonians

A new formulation to compute effective Hamiltonians for homogenization of a class of Hamilton-Jacobi equations is proposed. Our formulation utilizes an observation made by Barron-Jensen about viscosity supersolutions of Hamilton-Jacobi equations. The key idea is how to link the effective Hamiltonian to a suitable effective equation. The main advantage of our formulation is that only one auxiliary equation needs to be solved in order to compute the effective Hamiltonian $\bar{H}(p)$ for all p. Error estimates and stability are proved and numerical examples are presented to show very encouraging results.

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MS107

A Discontinuous Galerkin Method for Wave Propagation in Coupled Acoustic-Elastic Media

Our goal is to develop scalable methods for global full-waveform seismic inversion. The first step we have taken towards this goal is the creation of an high-order accurate discontinuous Galerkin method for simulation of wave propagation in coupled elastic-acoustic media. We use adaptive mesh refinement to resolve local variations in wave speeds with appropriate element sizes. The numerical accuracy and convergence of the method is studied for classical wave propagation interface problems.

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MS107

Accurate Numerical Methods for Waves in Very Heterogeneous Media

Abstract unavailable at time of publication.

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MS108

Finite Element Algebraic Multigrid Methods for Biomechanics of the Cellular Microenvironment in Articular Cartilage

We present a set of algebraic multigrid methods tailored to simulating inhomogeneous deformation in the biomechanical microenvironment of the cells in articular cartilage using the finite element method. 3D finite elements on unstructured meshes that conform to the shape of internal interfaces are employed. Applications that simulate the elastic deformation of soft cellular inclusions within an isotropic or transversely isotropic extracellular matrix will be discussed.

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MS108

Title Not Available at Time of Publication

Abstract unavailable at time of publication.

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MS108

Phase-field Model of Biofilm-flow Interaction

We derive a set of phase field models for biofilms using the one-fluid two-component formulation in which the combination of extracellular polymeric substances (EPS) and the bacteria are effectively modeled as one fluid component while the collective ensemble of nutrient and the solvent are modeled as the other. The biofilm is assumed an incompressible continuum. The dynamics of the biofilm is governed by a modified Cahn-Hilliard equation. Numerical simulations are carried out and biofilm growth, expansion, streaming, rippling, and detachment in shear cells are captured. Viscoelastic properties of the biofilm is investigated as well.

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MS108

Particle Alignment and Voronoi Tessellation of a

Sphere

We are interested in the orientation of non-spherical particles such as liquid crystal molecules, nanoparticles and colloidal particles due to interactions with each other and external fields. Since the orientation of a rod-like particle corresponds to a point on a unit sphere, the time evolution of the orientational distribution function typically corresponds to nonlinear diffusion on a sphere. Since the nonlinearity results in mode coupling, obtaining solutions in terms of spherical harmonics is not straightforward. We therefore turn to a direct discretization based scheme. Since in general it is not possible to construct a regular uniform lattice on a sphere, we construct a random lattice for our discretization. Two interesting problems arise in this approach. One is the identification of neighboring points on the sphere, required for the evaluation of derivatives; the other is the effective approximation of differential operators on a random lattice. To identify nearest neighbors, we construct the Voronoi diagram, using the Fortune sweep line algorithm which we have modified and adapted to be used on a sphere. To approximate differential operators, we have developed expressions for approximating the derivatives together with error estimates. In this talk, we give motivation for undertaking this work, discuss the first of the above two topics in some detail, and give examples implementing our strategy.

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MS109

High Order Finite Volume Wave Propagation with Application to Stegotons

We present a high order method for solving general hyperbolicproblems, based on wave-propagation form Riemann solvers, WENO reconstruction, and Runge-Kutta time integration. The method is very general in that it can be applied to systems with spatially varying flux or systems that are not in conservation form. The robustness and accuracy of the method are demonstrated through application to the study of solitary waves in a periodic non-dispersive medium.

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MS109

Radial Basis Function Methods Implemented using Extended Floating Point Precision - Examples, Insights, and Software

Radial Basis Function (RBF) methods often fail to realize their theoretical accuracy due to poor conditioning. We discuss how extended precision floating point arithmetic can be used to improve the accuracy of RBF methods in an efficient manner and use scattered data interpolation and steady PDE problems as examples. The effect of floating point precision on the eigenvalues stability of RBF methods for time-dependent problems will be examined. Software for implementing RBF methods with extended precision will be presented.

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MS109

Two Improved Algorithms for Stable Computations with "Flat" Radial Basis Functions (RBFs)

Smooth RBFs, which feature a free shape parameter, are receiving considerable attention for numerically solving PDEs since they combine high-order/spectral accuracy with meshless flexibility. Using shape parameters that produce "flat" RBFs typically lead to smaller discretization errors in applications. However, the direct numerical approach of computing with flat RBFs is severely ill-conditioned. We present two improved algorithms for bypassing this ill-conditioning, compare them to others presently available, and give some applications.

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MS109

A Phase-field Model for Two-phase Flows with Large Density Ratio and its Numerical Approximation

Modeling and numerical approximation of two-phase incompressible flows with different densities and viscosities are considered. A physically consistent phase-field model that admits an energy law is proposed, and several energy stable, efficient and accurate time discretization schemes for the coupled nonlinear phase-field model are constructed and analyzed. Ample numerical experiments are carried out to validate the correctness of these schemes and their accuracy for problems with large density and viscosity ratios.

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MS110

IMEX Runge-Kutta Schemes for Hyperbolic Systems with Stiff Diffusive Relaxation

Hyperbolic systems of conservation laws often have relaxation terms that, under a suitable scaling, lead to a reduced system of parabolic or hyperbolic type. The development of numerical schemes to solve systems of this form has an active area of research. Implicit-explicit (IMEX) schemes have been used for the time integration of such systems. Typically an implicit scheme is used for the relaxation term and an explicit scheme is used for the convection term. In this talk we will focus our attention to hyperbolic system of conservation laws with stiff diffusive relaxation. Usually these systems in addition to the stiff relaxation term have the convection term stiff too. We will mainly concentrate on the study of the stiff regime. In fact in the stiff regime most of the popular methods for the solution of these systems fail to capture the correct behavior of the relaxation limit unless the small relaxation rate is numericaly resolved. Other schemes present in the literature are able to overcome such a restriction, and relax to an explicit method for the underlying parabolic equations, thus suffering from the usual CFL stability restriction. Here we will show how to construct new IMEX schemes that overcome such difficulties by introducing additional *algebraic* order condition and maintain both the correct asymptotic limit (i.e., the correct zero-relaxation limit should be preserved at a discrete level) and the correct order of the scheme. Our findings are demonstrated on several numerical examples.

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MS110

Adaptive Mesh Refinement for Discontinuous Galerkin Schemes via Local Time-stepping

We present a strategy for adaptive mesh refinement for discontinuous Galerkin schemes that is based on unstructured conforming meshes. The main difference between our approach and the standard strategies commonly found in the literature is that we allow for a different time-step on each element. In this sense, the proposed method makes use of ideas from both the structured and unstructured approaches. The main advantage is that we are able to save computational effort by not taking small time-steps on coarse elements. The disadvantage is that interpolation in time must be applied in order to facilitate communication between elements. We present a variety of numerical examples to test the proposed numerical scheme.

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MS110

High-Order Simulation of Electrical Activity in Cardiac Tissue

Mathematical models of electric 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 method. In this talk, I relate our experiences with high-order numerical methods for the efficient solution of cardiac electrophysiological models.

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MS110

Implicit Integration Factor Methods for Spatial Discretization on High Dimensional Unstructured Meshes

Implicit integration factor (IIF) methods are a class of efficient "exactly linear part" methods for systems with both stiff linear and nonlinear terms. The challenge in applying IIF methods for high spatial dimensional problems is how to evaluate the matrix exponential operator. For spatial discretization of PDEs on unstructured meshes, how to efficiently apply the IIF temporal discretization was open. In this paper, we solved this problem by applying the Krylov subspace approximations to the matrix exponential operator. Then we apply this novel time discretization technique to Discontinuous Galerkin methods on unstructured meshes.

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MS111

Exploiting Vector Space Properties to Strengthen the Relaxation of Bilinear Programs. Application: Global Optimization of Process Networks

In this paper we present a methodology to find tight convex relaxations for a special set of quadratic constraints given by bilinear and linear terms that frequently arise in the optimization of process networks. The basic idea lies on exploiting the interaction between the vector spaces where the different set of variables are defined to tighten the relaxation of traditional approaches.

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MS111

Fast Summation for Non-linear Mixed-integer Optimization

By viewing the maximum of a function as the limit of certain sums or integrals, efficient summation / integration procedures yield approximation algorithms for optimization problems. We report on recent advances in exact integration, summation and mixed summation procedures for polynomial functions. The methods are related to Brion's formulas, exponential sums, Barvinok's intermediate valuations, and to the polynomial Waring problem (polynomials as sums of few linear forms).

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MS111

MINOTAUR: A New Solver for Mixed-Integer Nonlinear Optimization

We present a new package for solving mixed-integer nonlinear optimization problems, called MINOTAUR. MINOTAUR implements a range of branch-and-cut algorithms within a flexible object-oriented framework. We will comment on some software design issues and describe some recent work on tighter integrating nonlinear solvers into a branch-and-cut framework.

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MS111

Valid Inequalities and Convex Hulls for Bounded Multilinear Functions

We study the convex hull of the nonconvex set defined by a product of N variables, with bounds on each variable and on the product itself. (For n=2 and unbounded product, the classical McCormick inequalities define the convex hull, but less is known for more general cases.) We will discuss strong valid linear inequalities, motivated by the fact that many exact solvers for nonconvex optimization problems use polyhedral relaxations to compute bounds via linear programming. Time permitting, we will also discuss strong nonlinear inequalities for such sets.

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MS112

Compressive Sensing: a Paradigm Shift in Signal Processing

We survey a new paradigm in signal processing known as "compressive sensing". Contrary to old practices of data acquisition and reconstruction based on the Shannon-Nyquist sampling principle, the new theory shows that it is possible to reconstruct images or signals of scientific interest accurately and even exactly from a number of samples which is far smaller than the desired resolution of the image/signal, e.g., the number of pixels in the image. This new technique draws from results in several fields of mathematics, including algebra, optimization, probability theory, and harmonic analysis. We will discuss some of the key mathematical ideas behind compressive sensing, as well as its implications to other fields: numerical analysis, information theory, theoretical computer science, and engineering.

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MS112

Compressed Sending in Medical Imaging: Progress in Applications and Implementation

Compressed sensing has already stimulated lots of new research in MR imaging. Applications are already being delivered: for example in pediatric MRI we can speed up image aquisition from 8 minutes to 1 minute while maintaining diagnostic quality and confidence. This speedup is significant because children can actualy still still for one minute and the same equipment can be used many more times per hour. I will also discuss recent implementation advances on GPUs (ie processors originally developed for gaming) accelerating our reconstruction times from hours to seconds.

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MS112

Message Passing Algorithms for Compressed Sensing

Compressed sensing aims to undersample certain high-dimensional signals, yet accurately reconstruct them by exploiting signal characteristics. Accurate reconstruction is possible when the object to be recovered is sufficiently sparse in a known basis. Currently, the best known sparsity-undersampling tradeoff is achieved when reconstructing by convex optimization – which is expensive in important large-scale applications. Fast iterative thresholding algorithms have been intensively studied as alternatives to convex optimization for large-scale problems. Unfortunately known fast algorithms offer substantially worse sparsity-undersampling tradeoffs than convex optimization. We introduce a simple costless modification to iterative thresholding making the sparsity-undersampling tradeoff of the new algorithms equivalent to that of the corresponding convex optimization procedures. The new iterative-thresholding algorithms are inspired by belief propagation in graphical models. Our empirical measurements of the sparsity-undersampling tradeoff for the new algorithms agree with theoretical calculations. We show that a state evolution formalism correctly derives the true sparsity-undersampling tradeoff. There is a surprising agreement between earlier calculations based on random convex polytopes and this new, apparently very different theoretical formalism.

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MS112

Efficient Algorithms for Non-orthogonal Atomic Decompositions

Building on the success of generalizing compressed sensing to matrix completion, this talk discusses progress on further extending the catalog of objects and structures that can be recovered from few measurements. I will focus on a suite of data analysis algorithms designed to decompose signals into sums of simple atomic signals. I will show how to generically construct such decompositions and discuss which sets of atoms admit efficient decomposition algorithms with performance guarantees.

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MS113

A Stochastic Relationship between Fine and Coarse Scale Constitutive Parameters

One objective of current multiscale research efforts is to incorporate fine-scale information into coarse-scale constitutive laws in some "approximate' sense. This approximation necessarily introduces modeling error in the fine-to-coarse scale property relationship. The present work treats this relationship as a stochastic mapping and employs the maximum entropy principle to characterize this stochastic relationship by using fine-scale responses, that are also meaningful at the coarse level, as constraints for the coarse-scale responses.

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MS113

Efficient Algorithms for Computing Failure Probability

Computing failure probability is a critical step in many applications such as reliability based optimization. The most straightforward method is to sample the response space. This can be prohibitively expensive because each sample point requires a full scale simulation of the underlying physical system. The other approach is to adopt an accurate surrogate model for the system and sample the surrogate. This can be extremely efficient as long as one can construct such a surrogate. In this talk we demonstrate that a naive surrogate approach is fundamentally flawed, no matter how accurate the surrogate is. Furthermore, we present a hybrid algorithm that combines the surrogate and sampling approaches. The resulting method is accurate and much more efficient than direct sampling. Rigorous error estimate will be presented, along with numerical examples.

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MS113

Surrogate Driven Hazard Analysis

Creating hazard maps for large jurisdictions threatened by floods, landslides, debris flows involves physics models that are highly non-linear and have dimensions of the inputs and outputs that are both high subjecting us to a particularly acute form of the "curse of dimensionality". We describe here a solution methodology based on creating a fast surrogate computational solver using the output of the simulator as data for a Bayesian statistical model, which we refer to as an *emulator*. The simulator is run for a few hundred to few thousand inputs, an emulator is created, and re-sampling uses the emulator to generate desired statistics. For example, an emulator might be constructed from 1024 simulations, and a Monte Carlo sampling can then be performed using the emulator. We will describe here development of a hierarchical version of this methodology that enables parallel computation of the simulator runs and its use in generating a hazard map.

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MS113

Stochastic Dimension Reduction for Network Coupled Systems

Stochastic expansion techniques such as polynomial chaos provide a powerful means for propagating uncertainty in many types of nonlinear applications. However the cost of these methods becomes prohibitive when large numbers of stochastic variables are present. In this talk we investigate stochastic dimension reduction techniques for certain classes of network coupled systems that exploit their inherent structure to reduce the cost of the expansion. Applications of these techniques to nuclear engineering problems will be presented.

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MS114

Models of Influenza Dynamics with Mixing in a Cross-classified Population

In this talk I will present some preliminary results on influenza dynamics obtained by incorporating heterogeneous mixing among strata in a cross-classified population model. With the refinements in mixing, risks associated with particular outcomes of interest to policy-makers can be more reliably assessed from multiple stochastic realizations of the model.

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MS114

Mathematics of the 2009 Pandemic H1N1

I will present a model for the transmission dynamics of the novel influenza H1N1 pandemic in a population. The model, which stratifies the infected population in terms of risk of developing severe illness, will be rigorously analysed to gain insight into its dynamical features. The impact of mass vaccination on the disease spread will also be assessed.

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MS114
Mathematical Modeling of the Effectiveness of Facemasks in Reducing the Spread of Influenza

With limited supplies of antivirals and lack of effective vaccines, countries and individuals are looking at other ways to reduce the spread of novel H1N1. We construct and analyze a mathematical model in which a portion of the population wears a facemask during the pandemic. We conclude from our model that, if worn properly, facemasks are an effective intervention strategy in reducing the spread of novel H1N1.

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MS114
Responding to Pandemics in Real Time

I will discuss the challenges of allocating limited interventions for pandemic influenza given the limited and biased data available at the time decisions must be made, focusing on the types of data that are and are not available, and on methods to use those data as effectively as possible. Case studies will include two or more of: assessing severity, assessing transmissibility, and targeting interventions.

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MS115
Compressible Fluid Simulations Using OpenCL on Modern Architectures

OpenCL is a new framework for portable code development across accelerated and multicore computing architectures. This talk will cover some of the challenges encountered in developing a multiphysics solver for compressible fluid simulations using OpenCL. In particular, we will discuss several mid-level abstractions that we have developed to improve the accessibility of OpenCL for scientific applications developers.

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MS115
So You Want to Use a "Real" Equation of State

We discuss the algorithmic, numerical, and practical considerations needed to use general equations of state (EOS) in a hydrodynamic code. Such models raise a host of issues that must be addressed in a useful code. These include the implementation of the EOS's (e.g. analytic verses tabular), how material stiffness will affect the hydro solver, what happens when a material leaves the domain of its EOS, and how mixtures of materials can be treated.

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MS115
Front Tracking and its Coupling with Convection Dominated Problems

The renovated FronTier library, equipped with high order surface algorithms, is coupled with a set of new PDE solvers. This includes the AMR-enabling compressible solver, the incompressible Navier-Stokes solver and the precipitation solver. We apply these new solvers to simulations of fluid mixing, bubbling, jet, fluid-structure interaction and convection driven precipitation of subsurface flow. We will present some interesting verification and validation on these problems.

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MS115
The Piecewise-Parabolic Boltzmann Advection Scheme (PPB) for Multifluid Gas Dynamics

A new and powerful approach to multifluid hydrodynamics has been developed and applied to the turbulent mixing of fluids. The multifluid fractional volume variable is advected using the Piecewise-Parabolic Boltzmann (PPB) scheme, an extension to 3-D constrained advection of van Leer's Scheme VI for 1-D. Ten moments in each grid cell are updated by PPB in a strictly conserving formulation. Advantages of this approach and the results it delivers on multiple applications are discussed.

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MS116
Shallow Water Flow through Channels

The talk will discuss shallow water flows through channels of variable cross section. The equations model nearly horizontal flows, and may derived from the Euler equations by cross sectional averaging. They form a set of nonlinear hyperbolic conservation laws with geometric source terms. The presence of geometric source terms gives rise to a range of interesting flows including a variety of non-trivial equilibrium solutions. Recent years have seen a rapidly growing interest in development of numerical methods for shallow water systems. The talk will discuss a Roe-type upwind scheme for flows through rectangular channels, channels with trapezoidal cross sections, and channels with general cross section. General channel walls are approximated by piecewise linear segments, leading to piecewise trapezoidal cross sections. Conservation, near steady-state accuracy, velocity regularization and positivity near dry states will be discussed and results will be shown.

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MS116

A Pseudo-spectral Method with the Window Technique for Kadomtsev-Petviashvili Equation

In this talk, we will present a numerical method to study the initial value problem of the KP equation with certain initial waves. The numerical approach is based on the peuso-spectral method with a window technique to take care of the non-periodic condition at the computational boundary. We show that, for those initial waves, the solutions asymptotically converge to some of the exact solutions in a locally defined L2-sense.

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MS116

Streamline Visualization of Discontinuous Galerkin Solutions Using Smoothness-Increasing Accuracy-Conserving Filters

Visualizing streamlines obtained from discontinuous Galerkin (DG) approximations can be a challenging task due to the inter-element discontinuities. Recently, a smoothness-increasing accuracy-conserving filter has been applied as a tool to enhance the smoothness of the field and eliminate discontinuities between elements, thus resulting in more accurate streamlines. Additionally, it also increases the order of accuracy of the approximation from $\mathcal{O}(\langle^{\parallel+\infty})$ to $\mathcal{O}(\langle^{\in\parallel+\infty})$ for linear hyperbolic equations solved over a uniform mesh.

The two alternative strategies for filtering the discontinuous Galerkin method take into account filtering over the entire field as well as filtering along a one-dimensional streamline. The first implementation aids in the ability to use a less restrictive time integrator. This filtering is done in a tensor-product way. However, filtering near a boundary can become a problem. Additionally, this type of filtering can become expensive for computing solutions over multi-dimensional geometries. The second alternative involves filtering as the streamline integration is performed using Forward Euler. This filtering along a streamline allows for reduction in computational cost. However, in previous implementations an improved one-sided post-processor was needed as well as higher-order derivative information. In this presentation, we discuss how to improve both types of streamline filtering through the use of more accurate one-sided filtering as well as using higher order derivative information.

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MS116

Measures for Sensor Placement for Estimation of PDE Systems

The location of sensors is critical in the design of controlled systems. In this talk we describe different measures to aid in the placement of sensors (and actuators). In particular, functional gains and system radii, and discuss the computational challenges associated with these problems. For illustration purposes we consider the problem of estimating the temperature in a flow field through thermostats with the specific application to designing efficient control systems for high performance buildings.

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MS117

hp-Discontinuous Galerkin Method for Two-phase Flow in Porous Media

There is a need for efficient and accurate numerical methods for solving multiphase flow problems. In this talk, we show that high order discontinuous Galerkin methods are promising candidates. In particular, we consider two different formulations of the incompressible two-phase flow problems arising in porous media: ”phase-pressure, phase-saturation” formulation and ”global pressure, phase-saturation” formulation. We introduce implicit, fully coupled *hp*-schemes based on discontinuous Galerkin methods to solve numerically the two-phase flow problem. Numerical analysis (existence of the discrete solution, convergence) of the introduced schemes and simulations of the two-phase flow in homogeneous and heterogeneous media are presented.

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MS117

Analyzing HDG Methods like Mixed Methods

We present an analysis of HDG methods closely paralleling the analysis of mixed methods. Specifically, we construct a projection operator with certain weak commutativity properties, tailored to the structure of the HDG method. With this natural projection, the HDG method can be analyzed elegantly and transparently.

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MS117

An Efficient S-DDM Scheme for Compressible Flows in Porous Media

Porous media flows are important in many areas of science and engineering such as groundwater contamination modeling, environmental protection, and reservoir simulation, etc. The problems involve the physical features of the coupling, nonlinearity, convection dominance, large scale field and long term prediction. In this talk, for solving large scale compressible flows in porous media, we propose an efficient S-DDM scheme by combining the non-overlapping domain decomposition and the splitting technique. Numerical experiments are given to show the efficiency and accuracy of the S-DDM approach. The method takes the attractive advantages of both the non-overlapping domain decomposition method and the splitting technique, which reduces computational complexities, large memory requirements and long computational durations. The theoretical analysis of stability and convergence are also discussed in this talk. This is joint work with C. Du.

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MS117

Adaptive Discontinuous Galerkin Method for Contaminant Transport in Fractured Porous Media

Fractures play an important role in flow and transport processes through saturated and unsaturated geologic media. Because the permeability in fractures is generally greater than it in matrix by many orders of magnitude, fracture networks have the potential for being highly effective pathways for conducting fluid containing contaminant species. One challenge in numerical simulation of contaminant transport in this system arises from the dramatic difference of convection rates between the matrix and the fractures. In addition, the concentration in the matrix is also tightly coupled with it within the fractures by the molecular diffusion and mechanical dispersion in the transverse direction. To treat this problem effectively, adaptive spatial and/or adaptive temporal discretizations are necessary. In this talk, we will present adaptive discontinuous Galerkin method as applied to the simulation of the convection-diffusion-adsorption processes in cracked porous media.

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MS117

Discontinouos Finite Volume Element Methods for Darcy's Law

Motivated by the Crouzeix-Raviart finite elements, we develop nonconforming and discontinuous finite volume methods for the Darcy's equation. Numerical experiments will be presented. We shall discuss also comparison with the mixed finite element method and coupling with transport solvers. This is a joint work with Jiangguo Liu (ColoState) and Xiu Ye (UALR).

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MS118

OPAL, A Parallel Accelerator Simulation Framework for Present and Future Modeling Challenges

Abstract unavailable at time of publication.

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MS118

Efficient, High-Quality Image Contour Detection

Abstract unavailable at time of publication.

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MS118

An Embarrassingly Parallel Benchmark to Study Architecture Heterogeneity

Abstract unavailable at time of publication.

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MS118

Algebraic Multigrid for Multicore Architectures

Algebraic multigrid (AMG) solvers have proven to be extremely efficient on distributed-memory architectures. However, when executed on modern multicore cluster architectures, we face new challenges that can significantly harm AMG's performance. We discuss our experiences on various multicore architectures and present a set of techniques that help users to overcome the associated problems, including thread and process pinning and correct memory associations. We present results using both an MPI-only and a hybrid MPI/OpenMP model.

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MS119

Algebraic Multigrid for 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. This talk develops a nested-iteration-Newton-FOSLS-AMG approach to solve this type of system. 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. An algorithm is developed which uses the a posterior error estimates of the FOSLS formulation to determine how well the system is being solved and what needs to be done to get the most accuracy per computational cost. A reduced 2D time-dependent test problem is 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. This talk shows that this is achieved in a few dozen work units. (A work unit equals one fine grid residual evaluation.) In addition, a discussion of how the above methods relate to the energetics of the system will be given.

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MS119
Algebraic Multigrid on the GPU

Abstract unavailable at time of publication.

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MS119
Angular Multigrid Methods for Boltzmann Transport Equations

Beams of microscopic particles penetrating scattering background matter play an important role in several applications. Grid-based discretization of the governing Boltzmann transport equation leads to a very large system of algebraic equations, as the continuum solution itself is a function of many variables. We discuss an angular multigrid algorithm for a two-dimensional model problem, based on a careful choice of relaxation and coarse-grid correction processes. Numerical experiments show rapid, grid-independent convergence for typical electron-beam scattering.

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MS119
Algebraic Multigrid for Problems in Electromagnetics

Problems in electromagnetics are a challenge for algebraic multigrid solvers. The discrete operator is often complex-valued, indefinite, and non-self-adjoint, resulting in low-energy oscillatory error components. These oscillatory modes are not effectively handled by standard relaxation and coarsening procedures. We propose elements in the multigrid process that recognize the wave-like near null-space in the problem. Along with improved coupling information and more accurate interpolation, this results in a more robust method for scattering problems.

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MS120
Regularized Slender Body Theory

Various slender body theories allow for the representation of filaments in Stokes' flow by a distribution of fundamental solutions along the filament center line. We revisit the theory in the context of regularized forces in a small neighborhood along the center line. The regularization produces a smooth final expression that helps eliminate the computational instabilities of the unregularized formulas. The derivations of theories corresponding to those of Lighthill and of Keller and Rubinow are outlined. Consistency with these theories is verified and numerical examples are presented.

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MS120
Creep Ringing in Non-linear Viscoelastic Models

In rheometry, when a step stress is applied to certain materials, the initial response is an oscillating strain. These free oscillations arise form a coupling between the elasticity of the sample and the inertia of the apparatus. Studies using linear viscoelastic models have shown that analysis of this ringing can provide meaningful information of the coupling between micro-structure and bulk viscoelastic properties. In this work we extend those studies to non-linear models. We compare signature responses from several models and their relation to the sample's micro-structure.

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MS120
Flow Behavior in Sheared Biaxial Liquid Crystal Polymers

I will present a kinetic theory for flows of biaxial liquid crystals. This theory applies to both ellipsoidal and bent-core type nematogens. Phase behavior and phase transition in sheared biaxial liquid crystal flows will be discussed. In addition, rheological consequence and their dependence on the conformation of the nematogens will be presented as well.

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MS120
Are Viscoleastic Fluids Observable?

Observability is the ability to determine uniquely the state of the system from observable quantities. We apply the observability rank condition to study the observability of various viscoleastic fluids under imposed shear of extensional flows.

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MS121
Sensitivity Analsysis for Glucose Insulin Model

This talk we will presents a sensitivity identifiably analysis of a mathematical model of glucose insulin system. This model incorporates sufficient structure and complexity to allow for examining the metabolic action and regulation of glucose and insulin systems. The complexity of the model allows for the representation of a variety of modes and sites for action but at the same time the number of parameters renders the validation with accessible data problematic. Sensitivity identifiability techniques are employed to examine which parameters are mostly likely identifiable for a variety of potential sources of data on the state of the system. The information provided by this analysis allows

for a reasonable reduction in parameters to be estimated and can be used to consider which experimental tests might best allow for study of the control response patterns.

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MS121

Generalized Sensitivity Functions for Multiple Output Systems

Generalized sensitivity functions as introduced by K. Thomaseth and C. Cobelli can also be defined for multiple output systems and allow deciding if measurements for an additional output of a system may improve the quality of parameter estimates. It is also shown that generalized sensitivity functions provide a reasonable approximation of the partial derivatives of the estimated parameter vector with respect to the coordinates of the nominal or true parameter vector.

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MS121

Nonlinear Filtering and Parameter Estimation for Complex Biological Systems

Mathematical modeling plays an important role in studying complex biological systems and parameter estimation is an essential component of developing mathematical models. However, accurate estimation of parameters is computational challenging as high fidelity models can contain a large number of parameters. Nonlinear filtering is one method that can be used to sequentially estimate both the state and parameters. We shall examine the application of these filtering techniques on nonlinear models with varying sets of parameters.

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MS121

Modeling and Model Analysis of Nonlinear Viscoelasticity of Ovine Arteries

A better understanding of the biomechanical properties of the arterial wall can aid in the improvement of graft design and implementation. In this study we focus on the constitutive relationship of the arterial wall to describe the dynamic response of changes in cross-sectional vessel area induced by time-varying arterial blood pressure. We used inverse mathematical modeling on a 4-parameter Kelvin (linear) viscoelastic model and a 5&6 -parameter nonlinear viscoelastic models and tested them on in-vitro data from male Merino sheep. Parameter estimation, sensitivity and statistical analysis approaches were used to investigate and describe the viscoelastic vascular wall properties by allowing us to compare models and choose the most adequate one that enabled parameter estimation within physiological ranges.

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MS122

Towards Implicit Immersed Boundary/finite Element Methods

As part of a long-term research effort to develop realistic three-dimensional models of cardiovascular fluid-structure interaction (FSI), we have recently developed a new version of the immersed boundary (IB) method which allows for finite element (FE) representations of the elasticity of the immersed elastic structures. In this talk, I will provide an overview of this new IB/FE method and its application to cardiovascular FSI, and describe progress towards the development of an efficient implicit IB/FE method.

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MS122

A Multigrid Method for the Coupled Implicit Immersed Boundary Equations

In this talk a multigrid method for solving the linearized immersed boundary equations that arise in implicit time discretizations is presented. The method simultaneously solves the equations on the Eulerian and Lagrangian grids. Numerical tests which compare the efficiency of the method with an explicit-time method are presented for a variety of test problems. Analytical results are presented for simplifed model problems to provide insight into the success and limitations of the method.

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MS122

An Implicit Immersed Interface Method with the Velocity Decomposition Approach

The implicit time-stepping method that we present is based on the velocity decomposition approach, in which fluid velocity is split into a Stokes part, determined by the Stokes equations and the singular interfacial force, and a regular part, given by the Navier-Stokes equations with a body force resulting from the Stokes part. The immersed interface is advanced implicitly, using an approach that is cost-effective and does not require the iterative solution of a system of coupled nonlinear equations.

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MS122

The Use of Projection in the Immersed Boundary Method

This study focuses on the role of projection in the immersed boundary method. Analogous to how projection is used to enforce incompressibility, projection can also be used to meet the no-slip constraint. The present implicit approach requires no ad-hoc relations for determining the boundary force and can be extended to fluid-structure interaction problems. Techniques for accelerating the computation (nullspace method) and satisfying other physical constraints will be presented.

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MS123

Gradient-based Methods for Sparse Recovery

The convergence rate is analyzed for the SpaSRA algorithm (Sparse Reconstruction by Separable Approximation) for minimizing a sum $f(x) + \psi(x)$, where f is smooth and ψ is convex, but possibly nonsmooth. It is shown that if f is convex, then the error in the objective function at iteration k is bounded by $a/(b+k)$ for suitable choices of a and b. Moreover, if f is strongly convergence, then the convergence is R-linear. An improved version of the algorithm based on a cycle version of the BB iteration and an adaptive line search is given. The performance of the algorithm is investigated using applications in the areas of signal processing and image reconstruction.

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MS123

An Augmented Lagrangian Approach for Sparse Principal Component Analysis

Principal component analysis (PCA) is a widely used technique for data analysis and dimension reduction with numerous applications in science and engineering. However, the standard PCA suffers from the fact that the principal components (PCs) are usually linear combination of all the original variables, and it is thus often difficult to interpret the PCs. To alleviate this drawback, various sparse PCA approaches were proposed in the literature. Despite success in achieving sparsity, some important properties enjoyed by the standard PCA are lost in these methods such as uncorrelation of PCs and orthogonality of loading vectors. Also, the total explained variance that they attempt to maximize can be too optimistic. In this talk we propose a new formulation for sparse PCA, aiming at finding sparse and nearly uncorrelated PCs with orthogonal loading vectors while explaining as much of the total variance as possible. We also develop a novel augmented Lagrangian method for solving a class of nonsmooth constrained optimization problems, which is well suited for our formulation of sparse PCA. We show that it converges to a *feasible* point, and moreover under some regularity assumptions, it converges to a stationary point. Additionally, we propose two nonmonotone gradient methods for solving the augmented Lagrangian subproblems, and establish their global and local convergence. Finally, we compare our sparse PCA approach with several existing methods on synthetic, Pitprops, and gene expression data, respectively. The computational results demonstrate that the sparse PCs produced by our approach substantially outperform those by other methods in terms of total explained variance, correlation of PCs, and orthogonality of loading vectors. Moreover, the experiments on random data show that our method is capable of solving large-scale problems within a reasonable amount of time.

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MS123

Regularization Methods for Sum of Squares Relaxations in Large Scale Polynomial Optimization

We study how to solve sum of squares (SOS) and Lasserre's relaxations for large scale polynomial optimization. When interior-point type methods are used, typically only small or moderately large problems could be solved. This paper proposes the regularization type methods which would solve significantly larger problems. We first describe these methods for general conic semidefinite optimization, and then apply them to solve large scale polynomial optimization. Their efficiency is demonstrated by extensive numerical computations. In particular, a general dense quartic polynomial optimization with 100 variables would be solved on a regular computer, which is almost impossible by applying prior existing SOS solvers.

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MS123

A Derivative-free Regularized Trust Region Approach for Least-squares Minimization

We develop a framework for a class of derivative-free algorithms for the least-squares minimization problem. These algorithms are based on polynomial interpolation models and are designed to take advantages of the problem structure. Under suitable conditions, we establish the global convergence and local quadratic convergence properties of these algorithms. Promising numerical results indicate the algorithm is efficient and robust when finding both low accuracy and high accuracy solutions. Comparisons are made with standard derivative-free software packages that do not exploit the special structure of the least-squares problem or that use finite differences to approximate the gradients.

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MS124

Regularity of The Free Boundary in the Inverse First Passage Problem

We study the inverse first passage problem: Given a diffusion process $\{X_t\}_{t\geq 0}$ on a probability space (Ω, P) and a probability p on $[0,\infty)$, find a boundary, $x = b(t)$, such that p is the survival probability that X does not fall below b, i.e., for each $t \geq 0$,

$$p(t) = P(\{\omega \in \Omega | X_s(\omega) \geq b(s) \text{ for } \forall s \in (0,t)\}).$$

We show that when p is smooth and has negative slope, this viscosity solution, and therefore also the unique usc solution of the inverse problem, is smooth. Consequently, this viscosity solution furnishes a unique classical solution to the free boundary problem associated with the inverse first passage problem.

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MS124

Global Existence in Critical Spaces for Compressible Barotropic Viscoelastic Flows

We investigate the global existence of strong solutions to the compressible barotropic viscoelastic flow. The initial data are supposed to be close to a stable equilibrium with constant density. Using uniform estimates for an auxiliary hyperbolic-parabolic system with a convection term, we get the global well-posedness in a functional setting invariant with respect to the scaling of the associated equations. We also show a smoothing effect on the velocity, a L1 decay on the difference between the density and the constant reference state, and a L1 decay on the difference between the deformation gradient and the constant reference state.

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MS124

Energy Minimizers of a Thin Film Equation with Born Repulsion Force

We consider a singular elliptic equation modeling steady states of thin film equation with both Van der Waal force and Born repulsion force. We studied the corresponding energy minimizing solutions and their behavior as Born repulsion force tends to zero.

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MS124

Transonic Flow and Isometric Embedding

Transonic flows in gas dynamics and isometric embedding problem in geometry will be discussed. Their connection will be presented.

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MS125

Fast Sampling by Polynomial Acceleration

We give a new analysis that shows the equivalence of Gibbs samplers for normal distributions and the classical stationary iterative processes used to solve linear systems, that are now considered very slow. We establish a general form of this result, and then show how these samplers can be sped up appreciably by preconditioning and polynomial acceleration which are common acceleration techniques from numerical linear algebra.

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MS125

Couplings and Variance Reduction for MCMC

In this talk, I will explain how Markov couplings can be used to improve the accuracy of Markov chain Monte Carlo calculations in some situations where the steady-state probability distribution is not explicitly known. The technique generalizes the notion of control variates from classical Monte Carlo integration. The method will be illustrated using simple models of nonequilibrium transport. Time permitting, I will discuss extensions of these ideas to stochastic differential equations.

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MS125

Large-scale Stochastic Newton Methods for Statistical Inverse Problems Governed by PDEs

Abstract not available at time of publication.

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MS125

Multiscale Inversion Techniques for Flow in Porous Media

We present a statistical inversion technique for flow and transport problems in which measurements occur at different spatial scales. A Bayesian framework, employing a Karhunen-Loève representation of the material properties of interest, enables inference from sparse direct and indirect data. In particular, we explore multi-level Markov chain Monte Carlo algorithms aimed at improving the computational efficiency and accuracy of estimating multiscale permeability fields.

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MS126

Homo Psychologicus: Behavioral Aspects of Rational and Bounded Rational Epidemics

Recently, we have seen an increase in the use of theoretical models to reveal the subtleties of contact processes underlying the transmission mechanisms and the biological constraints of host-pathogen interactions. However, individual objective and subjective vulnerabilities to disease and their behavioral outcomes have been ignored. In this talk, we formulate a model of homo psychologicus's pathogen-avoidance mechanism and investigate aversive behavioral response to epidemiological events.

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MS126

A Sensitivity Matrix Based Methodology for Inverse Problem Formulation

We propose an algorithm to select parameter combinations that can be estimated using an ordinary least-squares (OLS) inverse problem formulation with a given data set. First, the algorithm selects the parameter combinations that correspond to full-rank sensitivity matrices. Second, the algorithm involves uncertainty quantification by using the inverse of the Fisher Information Matrix. Nominal values of parameters are used to explore the effects of removing certain parameters from those to be estimated using OLS procedures.

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MS126

Forecasting the Impact of Pandemic (H1N1) 2009 in the United

In this talk, I will discuss the results from a study that forecasted the impact of pandemic (H1N1) 2009 in the United States. The results indicated that the overall impacts of pandemic (H1N1) 2009 were mild and similar to seasonal influenza. However, unlike seasonal influenza, which usually targets the elderly, pandemic (H1N1) 2009 targeted school-age children.

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MS126

Epidemic Spread of Influenza Viruses: The Impact of Transient Populations on Disease Dynamics

The recent "swine flu" pandemic and "avian flu" outbreaks have brought increased attention to the study on the role of animal populations as reservoirs for pathogens that could invade human populations. Here, we study the interactions between transient and resident bird populations and their role on dispersal and persistence in the control of avian diseases. Our results show that mixing residents and migratory bird populations play an important role on the patterns of disease spread.

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PP1

Statistical Analysis of $La_{1-x}Sr_xCoO_{3-d}$ Perovskite Oxygen Vacancy Data

$La_{1-x}Sr_xCoO_{3-d}$ perovskite is an essential material for solid oxide fuel cells. How the oxygen vacancy concentration (d) changes with temperature, partial pressure, and

strontium content (x) determines the performance of the material. We have performed statistical analysis and inference on the extensive and scattered experimental values of d by developing code to visualize the data and applying weighted regression methods. Our model to predict d and our regression methods will be presented. Advisers: James Saal, Penn State; Jingyan Zhang, Penn State; Gregory Somers, State College Area High School; Qiang Du, Penn State; and Zi-Kui Liu, Penn State.

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PP1

Allosteric Regulation of Ribonucleotide Reductase: A Qualitative Model

We developed a qualitative mathematical model of the allosteric regulation of Ribonucleotide Reductase (RNR). Using a system of ordinary differential equations, we modeled the kinetic behavior of substrate production and regulation of RNR which utilizes two regulatory sites to modulate the outflow of the four types of dNDPs. The model reproduces and predicts behavior consistent with the enzyme's function in several special cases. Experiments designed to test the validity of the model are proposed. Advisers: Hongyu He and Naohiro Kato, Louisiana State University.

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PP1

A Modified Wilson-Cowan Model to Describe Mitral and Granule Cell Behavior in the Mouse Olfactory Bulb

We explore the behavior of mitral and granule cells in the mouse olfactory bulb using a modified Wilson-Cowan model. This model describes the average activity of excitatory and inhibitory neural populations. We have performed stability analysis and calculated bifurcation diagrams, power spectral densities, and leading Lyapunov exponents to study the effects of external excitation to the system. We furthermore define parameter regimes that quantitatively match experimental data relating to local field potentials in the bulb. Adviser: Matthew Valley and Stuart Firestein, Columbia University.

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PP1

Electrostatic Deflections of An Elastic Membrane

Surface tension and electrostatic forces have been observed in many physical systems. Now, with interest piqued by applications to many micro- and nanoelectromechanical systems (MEMS and NEMS), their study is more relevant than ever. Such systems that include the interplay of both forces become more complicated and compelling to analyze. In this talk, we explore recent theoretical work work in this area.

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PP1

A Boom Model: Trader Herding and Autocorrelation Through Communication

In this paper we study noise traders that communicate and trade with each other in a market. We begin by computing a statistic which identifies a boom, and use it on the NASDAQ-100 dot-com "bubble.' We next generalize the classical geometric Brownian motion stock model accordingly. We represent individual traders that observe each others' past n daily returns using a nonlinear vector autoregressive NLVAR(n) process. We model traders endogenously creating a market price. We measure autocorrelation and herding as functions of traders' communication level (α) and number of past daily returns (n) that the traders rely on. We find that autocorrelation and herding increase with communication level α, and they decrease with n. Under this model, we can specify α and n leading to traders forming spontaneous herds without specific leaders and thus to price booms. Finally we see that our model replicates the statistical property we examined of the NASDAQ-100 boom.

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PP1

Parallel Lagrange-Newton-Krylov-Schwarz Algorithms for Shape Optimization of Steady Incompressible Flows

We study parallel Lagrange-Newton-Krylov-Schwarz algorithms for two dimensional shape optimization problems governed by steady incompressible Navier-Stokes equations discretized by finite element methods on unstructured meshes. .A one-shot approach is introduced and the large KKT system is solved with a domain decomposition preconditioned Newton-Krylov method. The main focus is on the robustness of the method and the parallel scalability of the algorithms on supercomputers with a large number of processors.

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PP1

Modeling Sensory Input to the Lamprey Spinal Cord

We develop and evaluate a neural model of the lamprey's central pattern generator of locomotion, implemented as a chain of coupled oscillators. We simulate sensory input from edge cells, which measure the body's curvature, by forcing the chain at various positions, one at a time. Simulations that vary chain length, forcing position, and forcing connection strength have shown a monotonic increase in entrainment range as a function of forcing position along the chain. Advisers: Kathleen Hoffman, University of Maryland Baltimore County; Tim Kiemel, University of Maryland, College Park; and Eric Tytell, University of Maryland, College Park.

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PP1

Role of Transportation, Social Distance, and Delayed Vaccination on the Spread of A/H1N1 in Mèxico During 2009 (SIAM-WCD)

A metapopulation model was developed to investigate possible mecha-nisms underlying the different epidemic waves observed in Mexico during the novel swine origin influenza SOI-A/H1N1 pandemic of 2009. The model captures dynamics present in official data about the AH1N1 epidemic in Mexico. The model considers six different epidemiological classes: susceptible, incubating, infected but unconfirmed, infected and confirmed, recovered and vaccinated. The model allows the study of transient, and possibly random perturbations of the parameters in the model, thus enabling the study of possible scenarios and their different outcomes, but without restricting the dynamics to fixed rules. Populations were assumed to be arranged as a starred graph with center at Mexico City. The different populations were assumed to interact by means of land transportation. The effects of social distancing and school closures to the time course of the epidemic were investigated in conjunction with local transportation. Our simulations indicate that transportation alone does not explain the observed delays in the epidemic outbreaks for the different Mexican states. Nevertheless, a combination of local transport, and decrease in contact at specific dates during the year is sufficient to explain the different waves and general characteristics of the epidemic outbreak observed within Mexico. The numerical paradigm implemented to obtain the simulations for this model is suitable for other phenomena in which changes in the dynamics of the system change, whether or not randomly.

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PP1

Numerical Simulations Surfactant Spreading on Thin Liquid Films

Surfactant deposited on a liquid surface spreads due to imbalance of forces at its leading edge, acting on the liquid to create an expanding surface wave. Numerical simulations of this surfactant-liquid system are performed to explore how different initial conditions affect resulting wave dynamics. Both one- and two-dimensional regimes are considered. Data from numerical simulations is compared to experimental results. Adviser: Rachel Levy, Harvey Mudd College.

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PP1

A Simple Tonotopic Model of the Mammalian Auditory Pathway

This poster will show some interesting features of a simple tonotopic model of the auditory system in mammals. This is demonstrated with the frequency domain as well as through spectral content.

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PP1

Neuronal Bursting: Interactions of the Persistent Sodium and CAN Currents

Previous modeling efforts for individual neurons in the pre-Bötzinger complex have focused on either the persistent sodium current (I_{NaP}) or the calcium-activated nonspecific cationic current (I_{CAN}). Here, we analyze the effects of including both I_{NaP} and I_{CAN} within one model. Interestingly, we find that the presence of I_{NaP} enhances the ability of the cell to emit bursts featuring a period of depolarization block; previously, such bursts were only seen in the model with I_{CAN}.

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PP1

Anisotropic Phase Field Equations and Macroscopic Conditions

Recently [to appear in DCDS]we derived, from an integral form, an extended version of phase field equations of arbitrary order (for smooth interfaces with anisotropy) under the assumption that kernel (interaction potential) of the integral form consisted of finite sum of Fourier modes. We show that, even when the interaction kernel is only continuous, the same macroscopic quantities,in the asymptotic limit, are well defined and satisfy thermodynamic relations at the interface.

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PP1

Hybrid Asymptotic-Numerical Method for ODEs

Our research was motivated by the desire to develop an ODE solver that encapsulates the properties of the differential equation into a numerical method. We formulate a hybrid asymptotic-numerical method by incorporating the initial conditions into the differential equation so that we arrive at a better understanding of the local properties and their influence on the solution. Using dimensional analysis to scale the solution, we were able to formulate a novel approach to the solution that is extremely competitive with existing methods. Advisers: Raymond Chin and Giovanna Guidoboni, Indiana University-Purdue Univer-

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PP1

Vaccinating Against Hpv in Dynamical Social Network

We develop a dynamical network model to examine the relative merits of strategies for vaccinating women against the sexually transmitted Human Papillomavirus, which can induce cervical cancer. The model community is represented as a sexual network of individuals with links dynamically created and destroyed through statistical rules based on the node characteristics. Various strategies for distributing an allotted number of doses of vaccine are tested for effectiveness in reducing the incidence of cervical cancer.

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PP1

Analyzing a Gasdynamic System Via Characteristics

A wealth of analysis has been completed in applied mathematics involving physical models that incorporate combustion theory. In particular, much attention has been directed towards the modeling of reactive gasdynamic systems, which typically utilizes asymptotics. In this work we analyze such a system without the usage of asymptotics by considering a numerical estimate for a temperature function along a characteristic curve. We supplement this analysis with the development and implementation of a numerical procedure.

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PP1

A Stochastic Mortar Mixed Finite Element Method for Flow in Porous Media with Multiple Rock Types

We present an efficient multiscale stochastic framework for uncertainty quantification of flow through porous media. The governing equations are based on Darcy's law with nonstationary stochastic permeability represented as a sum of Karhunen-Loeve expansions, meant to represent multiple rock types. The approximation uses stochastic collocation on either a tensor product or a sparse grid, and couples it with a domain decomposition algorithm known as the Multiscale Mortar Mixed Finite Element Method. We employ a Multiscale Flux Basis, which reduces subdomain solves on each interface iterations to linear combinations of the basis functions, leading to a very efficient algorithm. Error analysis and numerical experiments are presented.

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PP1

Time-Optimal Control of Emergency Response Logistics: A Case Study

This paper begins the analysis of optimal control of emergency response logistics under a bioterror attack in the case of anthrax, which is a hybrid system consisting of a continuous-time dynamics and a resetting dynamics. The necessary conditions for time-optimal hybrid control are given, based on the calculus of variations and dynamic programming. To solve the hybrid Hamilton-Jacobi-Bellman equation, a wavelet-based approach is proposed. A gradient algorithm is implemented and used to test the queueing network model as well as the algorithm's own reliability. Experimental simulation results are presented and discussed.

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PP1

Sensitivity and Anisotropy in the Quasilinear Elliptic Non-Darcy Model

We consider several variants of the quasilinear elliptic non-Darcy model for flow in porous media. We are interested in the effects of anisotropy and in sensitivity to the model parameters such as powers of velocity and coefficients. In general, sensitivities to model parameters may not be well defined but in some cases we can express them in terms of known quantities. We also explore a coupled transport problem and discuss sensitivities in that problem.

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PP1

Applications of a Residual a-Posteriori Estimator for Coupled Elliptic and Parabolic Systems of Pdes

We consider systems modeling coupled flow and transport in subsurface and robust a-posteriori estimates for their finite element discretizations. The examples include classical Barenblatt model of double-diffusion as well as various models in which kinetic relationships replace equilibrium isotherms, or phase transition constraints. In particular we present modeling methane and carbon dioxide in coal beds and of methane hydrates. The estimator helps to construct an adaptive multilevel grid for each component of the system.

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PP1
Extensions of Sub-Linear Spectral Methods to Two Dimensions

We investigate spectral methods on sub-Nyquist grids using randomized and deterministic sub-linear time Fourier algorithms. These algorithms identify k of the most significant frequencies in the Fourier expansion of a given frequency-sparse signal of length $N \gg k$ and estimate their coefficients in $\mathrm{poly}(k, \log(N))$ time, using only a sub-linear number of samples. We extend previous results to two-dimensional Poisson and Helmholtz equations. Practical implementation issues are also discussed.

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PP1
An Investigation of An Inequality Involving Roots

In their aritcle, titled "Simple Trigonometric substitutions with broad results" on "Mathematical Reflections" journal, Campos Daniel and Verdiyan Verdan proposed an interesting inequality which had appeared in several occasions in MathLinks forum. In this paper, we will present two new solutions to this inequality problem. We also consider many generalizations to this inequality from different perspectives. Finally, we will apply the results to solve some other difficult inequality problems.

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PP1
Least-Squares Finite Element Methods for Incompressible Non-Newtonian Flow Problems

The goal of this work is to implement least squares finite element approaches for the equations governing non-Newtonian flows such those occurring in polymer processes and blood flow in arteries. By properly adjusting the importance of the mass conservation equation and a carefully chosen nonlinear weighting function, the least-squares solutions exhibit optimal L^2-norm error convergence in all unknowns or better in each dependent variable. Numerical solutions for flows through a 4-to-1 contraction channel will be considered. The effects of the viscosity, Weissenberg numbers are also investigated in the work

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PP1
Sound Source Separation via Tensor Decomposition with Sparse Factors

We present a new tensor-based numerical method for sound source separation. From a tensor data structure, each waveform of the musical instruments is obtained from a multi-channel signal mixtures. Our technique relies on ℓ_1 minimization for higher-order tensors. We demonstrate our algorithm on several music samples.

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PP1
AWM Workshop: Direct Sparse Deblurring

We propose a deblurring algorithm that explicitly takes into account the sparse characteristics of natural images and does not entail solving a numerically ill-conditioned backward-diffusion. The key observation is that the sparse coefficients that encode a given image with respect to an over-complete basis are the same that encode a blurred version of the image with respect to a modified basis. Following an "analysis-by-synthesis' approach, an explicit generative model is used to compute a sparse representation of the blurred image, and the coefficients of which are used to combine elements of the original basis to yield a restored image. We compare our algorithm against some state-of-the-art deblurring methods.

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PP1
AWM Workshop: Application of Population Dynamics to Study Heterotypic Cell Aggregations in the Near-Wall Region of a Shear Flow

This work focused on the modeling of polymorphonuclear neutrophils tethering to the vascular endothelial cells, and subsequential tumor cell emboli formation in a shear flow, an important process of tumor cell extravasation from the

circulation during metastasis. A population balance model is utilized, which for the first time, to our best knowledge, a multiscale near-wall collision model reconciles the effect of deformation on cell coagulation procedure, and works for general ratios of heterotypic cell.

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PP1

AWM Workshop: A Mathematical Model for the Spread of Animal Diseases in the United States with a Case Study on Rinderpest

Animal diseases are important in world economics, national security, and biodiversity. We create a spatially explicit, stochastic model for the spread of multi-host animal diseases in the United States with a case study of the highly virulent rinderpest. We explore geographical spread on a county level and different mitigation strategies. A forward sensitivity analysis indicates important disease parameters and containment approaches. Generalizations of control strategies for rinderpest may be effective for other contagious animal diseases.

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PP1

Optimal Strategies Under Limited Vaccination (SIAM-WCD)

The importance of preparing for influenza pandemics is critical. We devise optimal vaccination strategies in the face of limited vaccine doses by using a mathematical model of influenza transmission. The sensitivity of our results to varying certain epidemiological parameters including the basic reproduction number is studied. In particular, we study scenarios of unlimited and realistically limited vaccine scenarios. We introduce a constrained optimal control problem to construct different vaccination policies under different vaccine abundance. Finally our results suggest important public health recommendations, including a vaccine purchase quota so developed and developing countries can have the same access to vaccines.

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PP1

AWM Workshop: Fast Low Rank Approximations of Matrices and Tensors

A tensor is an object which extends the notion of scalars, vectors and matrices to multi-dimension. Modeling of real-world applications, result in automatic generation of very large data sets. Such data are often modeled as matrices: An m x n real-valued matrix A, provides a natural structure for encoding information about m objects, each of which is described by n features. However, other data needing more than two dimensions such as an m x n matrix changing with time requires a higher dimensional structure for encoding. Tensors which are the extension of matrices in higher dimension in such cases provide a good structure for encoding. Such data Tensors often have structural properties that present challenges and opportunities for researchers and as such, decomposing/factoring the data reveal some of these useful features. We shall consider the decompositions and approximation of a high definition image for compression. We shall offer other algorithms such as the FLRMA (Fast Low Rank Matrix Approximation) that approximates such decompositions with smaller computational cost. In addition, we shall analyze the numerical results and compare them to some other well know approximation schemes such as the Singular Value decomposition and a least square solver.

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PP1

Break-up of an Underwater Bubble: Singularity, Memory and Interference

Recent works revealed that dynamics near break-up of an underwater bubble does not evolve into a singular, universal form, independent of initial conditions. Instead, asymmetries in initial conditions excite vibrations in the neck shape that dominate the final break-up. We show that a model approximating the interaction between vibrational modes as linear interference gives outcomes in agreement with simulation results. Exceptions occur for initial states near threshold values for which the model predicts a qualitative change in final outcome. Adviser: Wendy Zhang, University of Chicago.

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PP1

The Role of Anti-inflammatories in Pattern Formation for Chemotaxis Models

The role of anti-inflammatories in pattern formation for chemotaxis models We study the spread and regulation of inflammation in the absence of specific pathogenic stimuli. We seek to understand the forms of rashes that occur due to the innate immune response. We incorporate anti-inflammatory cytokines into a reaction-diffsuion-chemotaxis model. Surprisingly, the incorporation of anti-inflammatories into the model encourages instability. Numerical simulations indicate show that if anti-infammatories are slow, our model can get moving and dynamic pattern formation whereas the current literature largely focuses on stationary patterns. Advisers: Bard Ermentrout and David Swigon, University of Pittsburgh.

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PP1

Mathematical Modeling, Analysis and Simulation of a Resonant Optothermoacoustic Sensor

Optothermoacoustic detection using a tuning fork receiver is a new technique for trace gas sensing with potential applications in environmental monitoring and medicine. The thermal source causes the receiver to deform which we model by coupling the heat and linear thermoelasticity equations. We study the effect of the source position on the generated signal and validate experimental results showing that the output is largest when the source is focused near the base of the receiver.

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PP1

Control of Milk Synthesis by Prolactin

Prolactin is a vital regulatory hormone secreted by the pituitary. This study focuses on the role of prolactin in the regulation of milk synthesis. A previous study described the creation of novel mathematical model of the regulation of the prolactin receptor during suckling. The current study focuses on expanding the knowledge surrounding the role of prolactin and its receptor using various modeling techniques.

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PP1

Mixed Convection in Cylindrical Annulus with Rotating Outer Cylinder and Radially Constant Magnetic Field

In the present study, mixed convection of a fluid in the fully developed region in horizontal concentric cylindrical annulus with different uniform wall temperatures is numerically investigated. The effects of radial MHD force as well as heat generation due to viscous dissipation are also taken into account. Buoyancy effect is also considered along with Boussinesq approximation. The forced flow is induced by the cold rotating outer cylinder in slowly constant angular velocity with its axis at the center of annulus. Investigations are made for various combinations of non-dimensional group numbers, Reynolds number (Re), Rayleigh number (Ra), Hartmann number (Ha) and Eckert number (Eck). Governing equations are continuity, two-dimensional momentum and energy.

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PP1

An Analytical Solution of Flow Between Two Rotating Spheres with Time-Dependent Angular Velocities

This research involves the study of an incompressible, Newtonian fluid flow between two concentric, rotating spheres with time-dependent angular velocities. The main purpose of the research is to study the use of an approximate analytical method for analyzing the transient motion of the fluid in the annulus. The governing equations are linearized by employing perturbation techniques. Then the meridional dependence in these equations is removed by expanding the dependent variables in a series of Gegenbauer functions with variable coefficients and using the orthogonality property of these functions. The equations for the variables coefficients are solved by separation of variables and Laplace transform methods. Results of the flow dynamics are presented for various Reynolds numbers up to 100. The results are presented for constant and time-dependent angular velocities.

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PP1

AWM Workshop: Local Existence and Uniqueness of Solutions to a Pde Model for Criminal Behavior

The analysis of criminal behavior with mathematical tools is a fairly new idea, but one which can be used to obtain insight on the dynamics of crime. In a recent work Short et al developed an agent-based stochastic model for the dynamics of residential burglaries. This model produces the right qualitative behavior, that is, the existence of spatio-temporal collections of criminal activities or “hotspots,’ which have been observed in residential burglary data. In this paper we prove local existence and uniqueness of solutions to the continuum version of this model, a coupled system of partial differential equations, as well a continuation argument. Furthermore, we compare this PDE model with a generalized version of the Keller-Segel model for chemotaxis as a first step to understanding possible conditions for global existence vs. blow-up of the solutions in finite time.

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PP1

How Large should a Forecast Ensemble be for a Complex Atmospheric Flow?

Complex geophysical flows typically are chaotic. That is, small uncertainties in initial conditions and localized instabilities grow exponentially in time. Currently, meteorologists use ensembles of initial conditions, at greater computational expense, to assess forecast uncertainties in a complex model. We seek to determine the minimum number of ensemble members needed to adequately resolve the multi scale dynamics in an idealized representation of an atmospheric jet using the Weather Research and Forecast-

ing (WRF) model. Adviser: Eric Kostelich, Arizona State University.

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PP1

AWM Workshop: Computational Aspects of Lie Algebras and Mubarakhzyanov Algebras

We investigate six-dimensional solvable Lie Algebras that have a five-dimensional nilradical. Such algebras were classified by the Russian mathematician G. M. Mubarakhzyanov in a paper published in 1963. The paper contains errors because calculations were done by hand and the list of algebras is incomplete. We make extensive use of MAPLE and some new routines to help finesse Mubarakhzyanov's list.

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PP1

Density-Dependence Effects in a Model of Persistent Bacterial Infections

Persisters are phenotypic bacterial variants which exhibit "antibiotic tolerance": persisters survive when exposed to bactericidal antibiotics, but the bacterial colonies regrown from persister cells remain susceptible to killing by further antibiotic treatments. Exactly how bacteria switch into a persister state is unknown, but persister formation is linked to quorum sensing (the ability of bacteria to detect the local population density). Persisters are also implicated in the formation and maintenance of biofilms, and they are believed to play an important role in chronic bacterial infections that resist antibiotic treatment. We present a reaction-diffusion PDE model of bacterial growth which incorporates nutrient- and population-density dependent mechanisms of persister formation. The functional form of this dependence is chosen to match experimentally observed relationships between nutrient availability, population growth rates, and incidence of persister phenotypes. These relationships involve a separation of temporal and spatial scales in the formation of persister vs. regular bacteria. We explore the effects of various experimentally accessible parameters related to quorum sensing on the rate and distribution of persister formation.

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PP1

Variance Reduction for Numerical Simulation of Stochastic Differential Equations

Stochastic differential equations arise in many applications including finance and materials. Since it is difficult to analytically determine their solution, we desire to minimize the error in our numerical approximations by reducing the variance of our estimator. Using the negative correlation properties of antithetic variates in conjunction with various numerical methods, we were able to reduce the variance of the estimators for the mean and variance of our approximations. This project was partly funded by the NSF CSUMS program.

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PP1

Gas Flow in Naturally Fractured Reservoirs: Numerical Solution of Restricted and Unrestricted Flows

Double porosity models are usually applied for naturally fractured reservoirs flow. It considers two regions: a low conductivity matrix, and high conductivity fractures. Beyond this, two types of flow from matrix to fractures are analyzed, restricted and unrestricted. In this work, these two flow kinds are numerically solved using finite difference and an implicit formulation including non-Darcy effects. The discretization scheme plays an important role in well flowing pressure features, especially in early times.

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PP1

AWM Workshop: A Mathematical Model of Glutathione Metabolism

Glutathione is produced by the liver and is highly important in neutralizing oxidative stress. Deficiencies have been correlated with a variety of diseases, including Down syndrome and autism. We have built a mathematical model of glutathione synthesis, transport, and break-down. We explore the half-life of glutathione and its sensitivity to fluctuations in amino acid input. Using the model, we simulate the metabolic profiles observed in Down syndrome and autism and compare the model results to clinical data.

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PP1

How to Find Relevant Patterns in Climate Data: An Efficient and Effective Framework to Mine Climate Time Series and Remote Sensing Images

This work presents a new unsupervised algorithm aimed at

discovering relevant patterns in climate and remote sensing time series. The patterns relate normal and abnormal behavior in data. This new algorithm works on multiple time series of continuous data, identifying relevant associations among the time series events. The associations can be visualized in a graphical manner, allowing a better identification and comprehension of the discovery patterns. Experiments over real climate data were performed. The results revealed patterns that the specialists described as not been known before and also interesting.

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PP1

Krylov Deferred Correction Embedded With Higher Order Methods

Spectral deferred correction was created to produce a deferred correction method of arbitrary order that was more stable than traditional deferred correction methods. This method was easy to implement as it used only first order schemes for prediction and correction. Krylov deferred correction was then created to accelerate spectral deferred correction. We are investigating using Krylov deferred correction embedded with higher order schemes and comparing the accuracy and efficiency against traditional Krylov deferred correction methods.

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PP1

AWM Workshop: Classification of Libs Protein Spectra Using Automatic Machine Learning Techniques

We performed multi-class classification of LIBS spectroscopy data which consists of samples from four proteins. We performed linear feature extraction by way of Principal Component Analysis (PCA). These features are used as inputs into the classification algorithms. We performed classification on LIBS data using the following classification algorithms: K-Nearest Neighbor, Classification and Regression Trees, Multi-layer perceptrons, Support Vector Machines, and Adaptive Local Hyperplane. We compared the classification accuracies of these algorithms using four-fold cross validation.

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PP1

Numerical Simulations of a Locally Forced Thin Film

We consider a model of a thin film of liquid on an incline driven by Marangoni forces induced by a temperature gradient. Localized forcing is included in the model. The effect of the forcing, which acts as a valve to constrain fluid flow is demonstrated. We describe the transient behavior of the system and the evolution of wave structures, including N-waves, as a result of the forcing profile and show agreement with the predictions of hyperbolic theory. Adviser: Rachel Levy, Harvey Mudd College.

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PP1

Coupling the Newton Dynamics and Aerodynamics of Insect Flight by the Immersed Interface Method

To study the stability and maneuverability of insect flight, we need to couple the Newton dynamics and aerodynamics. In this talk, I will present: (1) the formulas of the aerodynamic force and torque, (2) a matrix formulation of the Newton dynamics of a flying insect, and (3) coupling of the Newton dynamics and aerodynamics by the immersed interface method.

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PP1

AWM Workshop: Periodically Forced Hopf Bifurcation

We investigate the influence of frequency of a small periodic forcing on an ODE system near a point of Hopf bifurcation. The frequency of the forcing is close to the Hopf frequency. We use Liapunov-Schmidt reduction and singularity theory to find that the number of the forced periodic solutions can be sensitive to tiny changes of the forcing frequency. The full picture of bifurcation diagrams is obtained.

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PP1

Modelling Soil Erosion: Sediment Transportation

Modify the only multi size soil erosion model Hairsine-Rose model by considering the effects of sediment bedload and bed elevation. Composite Liska-Wendroff scheme (LwLf4) is used for solving the modified HR model. The numerical simulations are compared with MOL and experiment data under net erosion and deposition condition. Modified HR model is employed for solving 1-D buffer strip problem. The comparison of numerical approximations with experiment data shows good matches.

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PP1

AWM Workshop: Optimal Control of a Cholera Model

This work is to find an optimal vaccination rate that minimizes the economic and social losses in an ODE model of cholera. This model contains nine equations tracking movement of susceptible individuals with and without partial immunities. A vaccinated class and age structure are added into this model and the vaccination rate is a control function. Both analytical and numerical results are discussed.

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PP1

Dislocation Dynamics and PSB Formation

PSB (Persistent Slip Band) is believed to be the key inner configuration before crack initiation. Though many observations have been conducted to visulize it, few models could explane its formation. The law of motion for any single curve dislocation is proposed by considering the mobilities of edge and screw segment both. The stability analysis to rectilinear dislocation gives the critical orientation of a dislocation to cross slip. Then both numerics and asympotic analysis are applied to a planar dislocation curve, in order to find a critical stress for cross slip to happen.

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PP1

A Diffeomorphic Mean Curvature Flow for the Processing of Anatomical Surfaces

We introduce the diffeomorphic mean curvature flow, induced by restricting a diffeomorphic flow of Euclidean space to a surface. This flow has the potential advantage of being both topology-invariant and singularity free, which can be useful in computational anatomy for the processing of cortical surfaces. We derive an integro-differential equation for the flow, and describe numerical experiments on synthetic and cortical surfaces from neuroimaging studies in schizophrenia and auditory disorders.

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