IC1

An Overview of High Performance Computing and Challenges for the Future

In this talk we examine how high performance computing has changed over the last 10-year and look toward the future in terms of trends. These changes have had and will continue to have a major impact on our software. A new generation of software libraries and algorithms are needed for the effective and reliable use of (wide area) dynamic, distributed and parallel environments. Some of the software and algorithm challenges have already been encountered, such as management of communication and memory hierarchies through a combination of compile–time and run–time techniques, but the increased scale of computation, depth of memory hierarchies, range of latencies, and increased run–time environment variability will make these problems much harder. We will focus on the redesign of software to fit multicore architectures.

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IC2

Beyond the Human Genome Project: Challenges and Opportunities in Genomic Medicine

The sequencing of the human genome and the development of new methods for acquiring biological data have changed the face of biomedical research. The use of mathematical and computational approaches is critical to take advantage of this explosion in biological information. In this talk I will describe some recent discoveries resulting from the analysis of this data as well as their implications for the understanding and treatment of disease.

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IC3

Tensor Decompositions Solving Fundamental Problems in Chemistry

Tensor decompositions offer unique opportunities for solving problems that are otherwise impossible or very difficult to solve. In this talk we will present some recent applications and show how insight into the physics and chemistry can guide the development of suitable tensor models. The PARAFAC model, the PARAFAC2 model and constrained versions of these will be exemplified with various examples from systems biology.

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IC4

Complex Structures in Complex Networks

Graphs (or networks) of various kinds have found wide use in the biological, physical, and social sciences as convenient tools for representating of the topology of systems of interacting components. Understanding the structure of these networks is one of the outstanding challenges in the study of complex systems. Many simple forms of structure have been described and quantified, but it is possible for networks also to contain more complex structural features, including patterns and correlations on many different scales. This talk will describe some new methods for revealing structural features of networks in an automated fashion and give examples of their application to a variety of real-world networks.

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IC5

Depth-averaged Models and Software for Geophysical Flows

Many geophysical flows over topography can be modeled by two-dimensional depth-averaged fluid dynamics equations. The shallow water equations are the simplest example of this type, but it is often necessary to incorporate non-hydrostatic pressures, more complicated rheologies (e.g. for avalanches, landslides, or debris flows), or to use multi-layer models, e.g. for capturing internal waves or to model a landslide-induced tsunamis. These models are generally hyperbolic and can be modeled using high-resolution finite volume methods designed for such problems. However, several features of these flows lead to new algorithmic challenges, such as the fact that the depth goes to zero at the edge of the flow and that vastly differing spatial scales must often be modeled, making adaptive mesh refinement essential. I will discuss some of these applications and the GeoClaw software, a specialized version of Clawpack that is aimed at solving real-world geophysical flow problems over topography.

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IC6

A Stochastic Model of El Nino

Observations reveal that El Nio can be described by an almost embarrassingly simple model: a linear multivariate system driven by stochastic forcing. Such a model is able to reproduce properties usually associated with nonlinear properties, such as the preference of El Nio to peak in the boreal fall-winter, and the existence of fat tails in the probability distribution of sea surface temperatures (SSTs). In this talk, I will review the evidence that this simple model accurately describes the dynamics of sea surface temperatures in the Earth's tropical belt.

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IC7

Directions and Challenges in Web Search

Web search requires mapping an impoverished representation of a user's information need to a rich but incomplete representation of candidate units of content. I'll describe the trends in user behavior and in content creation that define the evolving shape of these two spaces. I'll also discuss the set of problems in web search that have received significant attention from the mathematics community, and the set of problems in web search that are deserving of mathematical treatment, and will argue that these two sets have some interesting differences.

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IC8

Challenges and Controversies in Multiscale Fluid Dynamics Algorithms for Numerical Weather Prediction and Climate Modeling

Climate and weather forecasting models contain: a "dynamical core" or "dy-core" that does the fluid mechanics. Dy-cores are now in a state of flux. The Old Reliable, a mixed spherical harmonic/finite difference algorithm, is near obsolescence. Finite volume, finite element, spectral element, finite difference and other algorithms are jousting for supremacy with no clear winner. Flow is strongly coupled across a range of length scales from planet-wide to little eddies that roil leaves in the lee of a house. Macroadaption — nesting a high-resolution regional model in a coarser global model — has been successful for hurricanes. Is microadaptation, which is refinement to track individual flow elements, feasible for flows so wavy? If it is, what's best on massivel-parallel supercomputers? We review the algorithmic agenda for constructing future climate oracles.

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IC9

Large Scale Inverse Problems in Imaging

Digital images are used to analyze objects in a variety of applications, such as star clusters in astronomy, molecules in biology, and tumors in medicine. Often postprocessing must be done to the collected data; this may involve reconstructing, restoring or enhancing the image. Mathematically these processes are modeled as inverse problems. Inverse problems usually cannot be solved analytically, and thus computational approaches must be used. In imaging, these computational problems are very large, requiring development of efficient solvers. Another difficulty is that the problems are very sensitive to errors, such as noise, in the data. This difficulty is usually handled by a technique called regularization. In this talk we describe some inverse problems that arise in imaging applications, approaches to regularize them, and our recent contributions to the development of iterative solvers.

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IC10

Mathematics of Olfaction

In this talk, I will discuss a number of interesting mathematical problems that arise in the study of olfaction, the sense of smell. The first gateway after the odor receptos is the olfactory bulb in mammals and the olfactory/antennal lobe in other animals. Oscillations are ubiquitous in this area and the mechanisms of their geneis and how they synchronize remain mysterious. In the first aprt of the talk, I will describe interactions of noise and oscillations as a means to synchronize rhythms in the bulb. I will then describe some other work on several mechanisms for the generation of these oscillations. Techniques from stochastic differential equations, bifurcation theory, and other nonlinear dynamics methods are applied to these questions. This is joint work with several graduate students and postdocs.

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IC11

Humane Data Mining

Data Mining has made tremendous strides in the last decade. It is time to take data mining to the next level of contributions, while continuing to innovate for the current mainstream market. We postulate that a fruitful future direction could be humane data mining: applications to benefit individuals. The potential applications include personal data mining (e.g. personal health), enable people to get a grip on their world (e.g. dealing with the long tail of search, enable people to become creative (e.g. inventions arising from linking non-interacting scientific literature), enable people to make contributions to society (e.g. education collaboration networks), data-driven science (e.g. study ecological disasters, brain disorders). Rooting our future work in these (and similar) applications, will lead to new data mining abstractions, algorithms, and systems.

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IC12

Large Scale Simulations of Earthquakes

Seismic waves due to earthquakes can be simulated through large scale numerical solutions of the elastic wave equation in the time domain. Some details of the numerical scheme will be described, which incorporates effects of distributed ruptures, heterogeneous elastic or visco-elastic materials, and topography. Examples will be given for some earthquakes in the San Francisco bay area, including the great 1906 San Francisco earthquake, which had a moment magnitude of 7.8-7.9. In the latter case, ground motions were calculated over a 550x200 kilometer area of northern California, measuring from the earths surface to a depth of 40 kilometers. These simulations used computational grids with up to 4 Billion points and the calculations were run on supercomputers at Lawrence Livermore National Laboratory.

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IC13

Graph Identification

Within the machine learning and data mining communities, there has been a growing interest in learning structured models from input data that is itself structured. Graph identification refers to methods that transform observational data described as a noisy, input graph into an inferred "clean" output graph. Examples include inferring organizational hierarchies from social network data, identifying gene regulatory networks from protein-protein interactions, and understanding visual scenes based on inferred relationships among image parts. The key processes in graph identification are: entity resolution, link prediction, and collective classification. I will overview algorithms for these tasks, discuss the need for integrating the results to solve the overall problem collectively.

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IC14

Large-scale Numerical Simulations of Fires and Explosion

With advances in high-performance computing, computer simulation is increasingly being used to augment theory and experimentation for scientific discovery and engineering analysis. However, many real- world scenarios require integration of a broad range of expertise, new computational methods, and a large quantity of computational power to achieve credible results that can be validated against theory and experiment. We discuss how these challenges have been approached in the Center for Simulation of Accidental Fires and Explosions (C-SAFE), a DOE-funded center involving several academic departments at the University of Utah. Explosive devices are both highly important and very common nationwide but present dangers to the general public. The primary purpose of C-SAFE is to develop insight into these materials and devices that will lead to improved methods for building, storing and shipping of hazardous materials. The driving scenario for C-SAFE is an explosive device (HMX in a steel container) engulfed in a hydrocarbon fire, proceeding from the ignition of the fire through the explosion of the device. Simulations of these events require successful integration of fluid mechanics, chemical reactions, and structural failure in time-scales ranging from tens of minutes to fractions of a millisecond. We employ a chemically reacting multiphase fluid-dynamics system, coupled with the Material Point Method (MPM) for simulating the massive deformations and fragmentation that occur during the rupture of the explosive device. We will discuss the Uintah software architecture that enables these simulations by providing a platform for integrating multiple parallel simulation components in a massively parallel application, which has also been used for modeling stage separation in rockets, growth of blood vessels (angiogenesis), and simulation of abnormalities in human vocal chords. In addition, we will show visualization tools that can examine several gigabytes of data simultaneously, or create pictures of a fire in a physically-based manner spanning from initial conditions to the final picture.

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IP0

Past President's Address: whydomath

One of the extraordinary and most satisfying features of mathematics is a kind of technology transfer that occurs when ideas developed in one field of mathematics apply equally well, and oftentimes in unlikely ways, in fields outside of mathematics. Katherine Socha and I have been leading a SIAM effort to develop a multimedia website, named whydomath, which will feature many success stories about the application of mathematics and computational science. The website, aimed at a freshman / popular science level, will be introduced at this meeting. Ultimately, whydomath will consist of many nodes, each one telling a story where the mathematical sciences has already proved instrumental in advancing an area of general societal interest, perhaps by being the foundation for a multi-billion dollar industry or, perhaps, just by providing the framework for unexpected advancement in another field. We want to highlight many of the ways in which the mathematical sciences have added value. In part the purpose of this talk is to present the website. But there is a more important goal: to challenge members of the SIAM community to help tell these stories.

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IP0

John von Neumann Lecture: The Effect of Local Features on Global Expansions

Global expansions, such as Fourier expansions, form the basis of many approximations which are successfully used in a wide variety of applications. Fourier expansions are used in applications ranging from medical CT scans, which are based on the Fourier expansion coefficients of an image, to spectral methods which are widely used to simulate complicated flows. While methods based on global approximations converge exponentially when the underlying function and all its derivatives are smooth, they lose accuracy in the presence of discontinuities. The term "Gibbs phenomenon" refers to the fact that the presence of a local discontinuity degrades the global convergence of such methods, although this fact was first pointed out by Albert Michelson. Over the years, a variety of techniques have been developed to alleviate or overcome the Gibbs phenomenon. These techniques include filtering (in the physical space as well as in the transform plane) and reprojections (re-expansing the numerical solution in a different basis). In this talk, we will present the history of the Gibbs phenomenon, and review the recent literature concerning overcoming of this phenomenon, including a discussion of methods for edge detection, which allow us to determine the location of the discontinuities.

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IP0

W. T. and Idalia Reid Prize in Mathematics Lecture: Numerical Methods for Two Geophysical Flow Problems

We very briefly describe recent work on two geophysical flow problems. First, we talk about analytical and computational results for a coupled Stokes-Darcy model related to flows in karst aquifers, where the coupling is effected using the full Beaver-Joseph interface conditions. Then, we talk about novel unstructured meshing techniques and corresponding discretization methods for oceanic flows.

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IP0

The AWM-SIAM Sonia Kovalevsky Lecture: A Noisy Adiabatic Theorem: Wilkinson Meets Schrdinger's Cat

The adiabatic theorem gives conditions that guarantee that a system defined by Schrdinger's equation remains in its ground state when started in its ground state and evolved slowly. Realistically, such systems are subject to perturbations in the initial condition, systematic time-dependent perturbations in the Hamiltonian, coupling to low-energy quantum systems, and decoherent time-dependent perturbations in the Hamiltonian. Using Wilkinson-style perturbation analysis, we derive bounds on the effects of these perturbations. This is joint work with Michael J. O'Hara.

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IP0

I.E. Block Community Lecture: Stylish Mathematics

All too often we see mathematics and the arts as two sides of the science/humanities coin. In this talk we'll see a place in which the two come naturally together in exciting new research. For in today's world in which almost all aspects of life are brought to the common medium of the computer, it is now possible to quantify and extract the style of an artist via computation. Examples are gleaned from the literary, visual, and dance arts, and include applications to the problem of authentication as well as to the more general problem of quantifying one's personal style. Taken together, this body of work shows just how "stylish" mathematics can be!

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IP1

The Geography of Social and Information Networks

The growth of on-line information systems supporting rich forms of social interaction has made it possible to study social network data at unprecedented levels of scale and temporal resolution. This offers an opportunity to address questions at the intersection of mathematics, computing, and the social sciences, where mathematical models and algorithmic styles of thinking can help in formulating models of social processes and in managing complex networks as datasets. We will discuss some of the emerging questions in this area, including the problem of tracking and modeling how information, ideas, and influence spread through large social networks, and the technical challenges in reasoning about privacy and personal data in a world where almost every transaction is recorded.

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IP2

Tensor Computations and Applications in Data Mining

Analyses of data organized as matrices are ubiquitous and well supported by theory and algorithms. In many applications data are organized in more than two categories, and it is often unnatural to reorganize the data as a matrix. Thus there is a need for theory and algorithms for tensor computations. In fact, tensor methods have been used in psychometrics and chemometrics for four decades, but it is only in recent years that the numerical linear algebra community has become interested in the area. The singular value decomposition (SVD) is a standard tool for analysis and computations in many applications. We discuss possible generalizations of the SVD for tensors, in particular those related to the best low-rank approximation property of the SVD. A few algorithms for computing the best low-rank approximation of a tensor are described, and we also point at unsolved theoretical problems. Finally the use of tensor methods in a couple of areas in data mining is illustrated.

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IP3

Software Design for Scientific Applications

Software development in scientific research environments poses many significant and conflicting challenges. Research environments (and their associated drive to publish! publish! publish!) require rapid and flexible software development that simplifies experimentation with new algorithms and data structures. Simultaneously, for our work to impact a broader community, we must create nearly production-quality software, as well as provide user support and code maintenance. With these conflicting demands (and, often, shrinking budgets), the right balance between research and software development is difficult to define. This talk will discuss these issues and suggest software design solutions that can ease the burden of software development in a research environment. Examples will be drawn from the Zoltan and Trilinos toolkits, as well as Sandia's new PDE Rapid Development effort and the SciDAC ITAPS (Interoperable Technologies for Advanced Petascale Simulations) project.

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IP4

Methods for Using Protein Interaction Networks to Interpret the Effects of Natural and Prescribed Genetic Variations

Physical and genetic mapping data have become as important to Network Biology as they were to the Human Genome Project. Physical interaction maps are being constructed through systematic measurements of protein-protein, protein-DNA, and protein-small molecule interactions. Genetic interaction maps are being generated by large-scale screening of synthetic-lethals and epistasis, by multipoint gene association studies, and by mapping the effects of natural and prescribed genetic variations on gene expression. We are working on methods and models for integrating physical and genetic interaction maps to assemble models of gene regulatory pathways. These efforts face several challenges, including: increasing the coverage of each type of network; establishing methods to assemble individual interaction measurements into contiguous pathway models; and annotating these pathways with detailed functional information. Efforts in each of these areas will be described. Using integrative tools, we are constructing network models to explain the physiological response of yeast to DNA damaging agents.

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JP1

The Heat Equation with Us Forever

What good comes from applying the heat equation to a digital image? The obvious answer is nothing: the heat equation just mixes colors and blurs images. Likewise could a solution to the Laplace equation produce decent images? Again, the a priori answer is no since a solution to the Poisson equation is smooth, and hence results in blurriness. Contradicting this doxa, I'll show that long-pursued aims in image processing and in image analysis are solved with the simplest linear PDEs: the heat equation and the Poisson equation. Three examples are treated. All three are basic questions about images and their perception. Thus, one could do a crash course in image processing with just the Laplacian. In the talk I'll go over such a course. The first problem is shape recognition. A recent algorithm invented by David Lowe gives an wonderfully complete solution. At its core lies the heat equation. The second example is Land's retinex theory, which delivers optimally contrasted images. Lo and behold the restored image is the solution of a Poisson equation! My third example is image denoising. Untold methods have been suggested for this puzzling problem, including all sorts of nonlinear heat equations. Yet the problem is elegantly solved by the heat equation.

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CP1

Analysis of a Drug-Drug Interaction Problem from Pharmacokinetic

A two drug interaction is usually predicted by individual drug pharmacokinetic. An improved drug-drug interaction prediction method based on a three-level hierarchical Bayesian meta-analysis model uses Monte Carlo Markov chain (MCMC) pharmacokinetic parameter estimation procedure. Underlying the present one is a fast integration method of the stiff pharmacokinetic equations. We report the establishment of the existence-uniqueness of the solution and the interaction between the MCMC procedure and the numerical integration scheme.

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CP1

Modeling Shrimp Biomass and Viral Infection for Production of Biological Countermeasures

We consider a novel approach for developing a stable operational platform for the rapid production of large quantities of therapeutic and preventive countermeasures. To this end, we present a size and class-age structured biomass/epidemiological model and corresponding numerical simulations. We couple equations for biomass production with those for vaccine production in controlled shrimp populations that have been infected with a recombinant viral vector expressing a foreign antigen, such as the Taura Syndrome virus.

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CP1

A Discrete Optimization Formulation and Analysis for the General Minimum Cost Vaccine Formulary Selection Problem

As the complexity of the United States Recommended Childhood Immunization Schedule increases, a combinatorial explosion of choices is being presented to public health policy makers and pediatricians. A discrete optimization problem, termed the General Minimum Cost Vaccine Formulary Selection Problem (GMCVFSP), is presented, which models a general childhood immunization schedule. Exact algorithms and heuristics for GMCVFSP are discussed. Computational results are also reported. The results reported provide fundamental insights into the structure of the GMCVFSP model.

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CP1
Classification and Regression Tree in Prediction – Case of Curative Gastrectomy Using Clinical Factors

This study was conducted to model the in vivo angiogenesis parameter – Color Doppler vascularity index (VI) by assessing the predictive value of regular molecule factors through the classification and regression tree methods. The optimal tree resulting was determined by receiver operator characteristic curve area. Among the molecule parameters, the most contributions were selected to the classification of high and low VI of gastric cancers. The predictive VI used to test the prediction of angiogenesis and prognosis in an independent group by using nonparametric testing of bootstrap resample.

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CP1
Optimal Control Applied to Native-Invasive Population Dynamics

An ODE system modeling interactions between invasive and native species is presented. Disturbance in the system is modeled as a control variable in the growth terms. An objective functional is formulated to maximize the native species while minimizing the cost of implementing the control. A new existence result for an optimal control in the case of quadratic growth functions is given. Numerical results provide suggestions for managing the disturbance regime when invasive species are present.

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CP1
Modeling the Sleep/Wake Cycle

A model of the human sleep/wake cycle that consists of a system of integro-differential equations describes the behavior of inhibitory and excitatory neurons contributing to the function of sleep regulating brain regions. We utilize properties of the REM/NREM cycle as well as stability theory and computational methods to analyze the system. A correlation is shown between the models output and experimental data as well as previously established knowledge of human circadian processes.

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CP1
Pattern Formation in the Gierer-Meinhardt model with parameters varying in space and time

This talk focuses on a reaction-diffusion system modeling pattern formation in developmental biology (morphogenesis). Optimal control theory is used to find the parameters that lead to patterns mimicking those found in nature, which is an improvement on the common ad hoc approaches applied previously. The basic approach is to minimize a cost functional that measures the discrepancies between a given state called the 'target', in this case a pattern found in nature, and the solution of the reaction-diffusion system. The parameters of the system are treated as distributed controls. The results of some numerical experiments in 2-D are presented using the finite element method, which illustrates the convergence of a variable-step gradient algorithm for finding the optimal controls of the system.

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CP2
Deriving Componentwise Condition Numbers Using Dual Techniques. Application to Linear Least Squares.

In perturbation analysis for linear algebra problems it is sometimes more appropriate to use componentwise or column/row-wise norms to measure perturbations in matrices, especially when the problem is badly scaled. Following a recent work on normwise condition numbers, we propose the use of dual norms and adjoint operators to derive closed formulas for componentwise and column/row-wise condition numbers. We apply this techniques to linear least squares and detail how to compute these quantities using Sca(LAPACK).

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CP2
Reorthogonalization for Accurate Singular Values

in Lanczos Bidiagonal Reduction

Lanczos bidiagonal reduction generates a factorization of a matrix $X \in \Re^{m\times n}, m \geq n$ such that

$$X = UBV^T$$

where $U \in \Re^{m\times n}$ is left orthogonal, $V \in \Re^{n\times n}$ is orthogonal, and $B \in \Re^{n\times n}$ is bidiagonal. Since the Lanczos recurrance tends to lose orthogonality, a reorthogonalization strategy is necessary to preserve convergence of the singular values of the leading $k \times k$ submatrix $B_k = B(1{:}\,k, 1{:}\,k)$ to those of B. Moreover, in the solution of ill-posed least squares problems and in the computation of matrix functions it is essential that this convergence occur properly. It is shown that if

$$\eta(V) = \|I - V^T V\|_F$$

then singular values of B correspond to those of X according to

$$|\sigma_j(X) - \sigma_j(B)| \leq O(\varepsilon_M + \eta(V))\|X\|_2$$

where ε_M is machine precision. Moreover, if

$$\Theta_1 = \mathrm{diag}(\theta_1, \ldots, \theta_\ell)$$

are the leading ℓ singular values of B_k then the corresponding approximate left singular vectors of X in the matrix P_ℓ satisfy

$$\|I - P_\ell^T P_\ell\|_F \leq O(\varepsilon_M + \eta(V))\|X\|_2/\theta_\ell.$$

Thus regulation of the orthogonality of the columns of V serves to preserve accuracy in the singular values and orthogonality in the leading approximate left singular vectors.

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CP2

Coupling Informatics Algorithm Development and Visual Analysis

We present a new visualization application used in developing informatics algorithms based on vector space models of data. Visualization of the data analysis results has led to better understanding of the overall impact of different parameters of several existing algorithms. A description of the system along with an example highlighting the application of the new tool to the development of a set of algorithms based on latent semantic analysis will be presented.

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CP2

A Poisson Solver Based on Iterations of a Sylvester System

We present an iterative scheme for solving Poisson's equation in 2D. Using finite differences, we discretize the equation into a Sylvester system $AU + UB = F$ involving tridiagonal matrices A and B. The iterations occur on this Sylvester system directly after introducing a deflation-type parameter that enables optimized convergence. Analytical bounds are obtained on the spectral radii of the iteration matrices. Our method is faster than SOR and amenable to compact programming via vector/array operations.

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CP2

Coefficients of Ergodicity and Eigenvalue Bounds

Coefficients of ergodicity measure the rate at which products of stochastic matrices, especially products whose number of factors is unbounded, converge to a rank-one matrix. Ergodicity arises in the context of Markov chains and signals the tendency of the rows of such products to equalize. We present simple definitions for coefficients of ergodicity for stochastic matrices, extend their definition to general complex matrices, and illustrate their connection to eigenvalue inclusion regions.

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CP2

Inexact Krylov Subspace Methods for PDEs and Control Problems

When a known good preconditioner is not easily computable, one can approximate it. This approximation may be accomplished with an iterative method. One question is how accurately to solve the (inner) iteration. In our work on Inexact Krylov methods, we have shown that the inner iterations can be solved progressively less accurately, as the underlying Krylov method (e.g, GMRES) converges to the overall solution. We discuss these criteria, and illustrate its application to several problems. In particular, we report on applying these ideas to parabolic control problems, where the reduced Hessian has two different inverses; and thus two inner iteration criteria are needed.

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CP3

Simulated Two-Dimensional RBC Motion, Deformation, and Partitioning in Microvessel Bifurcations

Red blood cell (RBC) motion, deformation, and partitioning in diverging microvessel bifurcations are simulated using a two-dimensional, flexible-particle model. Significant deviations of RBC trajectories from the streamlines of the fluid flow result from RBC migration towards vessel centerlines and from RBC obstruction of downstream vessels.

The effects of these behaviors on partitioning of RBCs in symmetric and asymmetric bifurcations are predicted and compared with experimental results.

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CP3

Understanding Dynamics of Gene Regulation Using a Discrete Model

Traditionally gene regulation is modeled by ordinary differential equations and the solutions are tested against experimental data. R. Laubenbacher and his group the Virginia Bioinformatics Institute are working on a discrete model that gives insight to the dynamics in gene regulation. We investigate the molecular mechanisms as a time-discrete finite dynamical system and compare the output with a continuous model.

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CP3

Quantifying Intermittent Transport in Cell Cytoplasm

Active cellular transport is a fundamental mechanism for protein and vesicle delivery, cell cycle and molecular degradation. Viruses can hijack the transport system and use it to reach the nucleus. Most transport processes consist of intermittent dynamics, where the motion of a particle, such as a virus, alternates between pure Brownian and directed movement along microtubules. In this communication, we estimate the mean time for particle to attach to a microtubule network. This computation leads to a coarse grained equation of the intermittent motion in radial and cylindrical geometries. Finally, by using the degradation activity inside the cytoplasm, we obtain refined asymptotic estimations for the probability and the mean time a virus reaches a small nuclear pore.

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CP3

Using Toxicokinetic Data to Develop Model Predictions for 4-Methylimidazole Chronic Exposure

4-methylimidazole (4MI) is a chemical that has been under investigation by the National Toxicology Program. A physiologically based pharmacokinetic model representing the uptake, distribution, and metabolism of 4MI in rodents was developed to describe the processes involved in 4MI toxicokinetics. Several model parameters did not have literature estimates; these were estimated by least squares techniques. The model was fit to short timespan data. The fit model was used to predict plasma concentrations of 4MI in multi-month feed dose study.

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CP3

Self Assembly of Dendritic Molecules Using Molecular Dynamics

Molecular self-assembly (without the intervention of external forces) is essential to the functioning of cells, molecular nanotechnology to construct objects at the nanoscale and micro scale cells. For example, self-assembly of lipids to form the membrane, the formation of double helical DNA through its hydrogen bonding of the individual strands, and the assembly of proteins to form quaternary structures. Molecular self-assembly of incorrectly folded proteins into insoluble amyloid fibers is responsible for infectious neurodegenerative diseases and many more. It is an important factor to understand its process in many applications. Therefore, molecular dynamics equilibrium statistical-mechanical calculations via simulation, is being proposed to study such phenomena. Simple vibrations, like bond stretching and angle bending, give rise to Infra-red spectra, NMR chemical shift and atomic force microscopy atomic indentation. Chemical reactions, hormone-receptor binding, self assembly and other complex processes are associated with many kinds of intra- and intermolecular motions. Here we will present a useful numerical simulation of the self- assembly of tree-like structure (dendrimers) of molecules under various acidic solvent.

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CP3

A Mathematical Model for Calcium Regulation in Yeast Cells

In eukaryotic cells, one of the functions of calcium is to serve as an intracellular messenger in response to extracellular factors. We present a model for the regulation of cytosolic calcium concentration (calcium homeostasis) in yeast cells. The model considers sequestration into the endoplasmic reticulum and vacuole as the regulatory mechanisms. We study the equilibration of internal calcium concentration after an external concentration change and discuss the stability of the final equilibrium state

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CP4

A Computing Technique to Accelerate the Convergence of Some Restarted Projection Methods

We propose a technique to improve the convergence of implicitly restarted Arnoldi method for calculating some eigenpairs of large sparse non Hermitian matrices. This approach is based upon to the projection of a large eigenproblem to several subspaces and to make use of their intermediary results for accelerating their convergence. We show that this technique can be extended to restarted projection methods for linear algebra problems and establish its interest for large-scale distributed computing.

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CP4

Enhancement of Krylov Subspace Spectral Methods by Block Lanczos Iteration

This talk presents a modification of Krylov Subspace Spectral (KSS) Methods, which build on the work of Gene Golub and others pertaining to moments and Gaussian quadrature to produce high-order accurate solutions to variable-coefficient time-dependent PDE or systems of PDE. The modification uses block Lanczos iteration to compute each component of the solution. Numerical results suggest that block KSS methods are significantly more accurate than their non-block counterparts, and also possess highly favorable stability properties.

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CP4

A Novel Parallel Hybrid Linear System Solver

Many realistic, multiphysics-multiscale, simulations in computational science and engineering give rise to very large sparse linear systems that need to be solved efficiently on parallel petascale architectures. Direct solution of these systems is often not possible due to memory limitations and poor scalability on massively parallel platforms. In these cases, one resorts to preconditioned iterative solvers. Unfortunately, unless the preconditioners are motivated by the specific application, these preconditioned schemes are not robust and lack the reliability of direct solvers. In this presentation we describe an alternative parallel hybrid approach for the solution of large sparse linear systems. It consists of the following general steps. First, the linear system is reordered into a banded form, sparse within the band, or low-rank modification of a central band. This can often be achieved by a reordering scheme such as reverse Cuthill-Mckee, weighted spectral or minimum cut. Second,the system is partitioned as a set of overlapped diagonal blocks. These blocks are all dependent on a small balance system, which is not formed explicitly, but can be solved via a modified preconditioned iterative scheme that requires the direct solution of those individual diagonal blocks. Once the balance system is solved the overall solution is retrieved with almost perfect parallelism. This work expands on the approach used in [M. Naumov and A. Sameh, "A Tearing-based Parallel Hybrid Banded Linear System Solver", submitted to J. Comp. and Appl. Math., Jan. 2008] for banded matrices. Numerical experiments will be presented.

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CP4

Hybrid Asynchronous Preconditioned Gmres Methods on a Nation-Wide Grid

In order to solve very large linear non-Hermitian sparse systems, we may start to compute Ritz elements to optimize the computation of a polynomial which will accelerate the convergence of restarted GMRES methods. The Arnoldi method is use to compute the Ritz elements in parallel of the GMRES iterations. Ritz elements are periodically sent to the GMRES process with respect to their accuracies and subspace sizes. These two methods are asynchronously interconnected and we distributed them on a large Nation-Wide cluster of clusters. We will present results obtained on GRID5000 for large sparse matrices with respects to several parameters such as the subspace sizes of the two methods. We will conclude with an analysis about hybrid linear algebra methods on such nation-wide grids.

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CP4

Blocked Sparse R-Bidiagonalization Using Givens Rotations

Computing the Singular Value Decomposition of sparse matrix requires bidiagonalization of a sparse upper triangular matrix R. We present two novel methods that use a sequence of Givens rotations to bidiagonalize R while exploiting sparsity. We introduce two variations of a dynamic blocking scheme which will generate the same amount of fill as the scalar version. We also discuss preliminary results towards a symbolic factorization and performance results comparing all the methods.

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CP5

Residuum-Correction Formulation of the Multi-Scale Finite-Volume Procedure

The multi-scale finite-volume procedure (MSFV, Jenny et. al, JCP 2003) for the approximated solution of elliptic problems with variable coefficients has been recently developed to an iterative procedure allowing convergence to machine accuracy (Hajibeygi et. al., submitted JCP). We propose further improvements to ensure solvability, when the coefficient varies over many orders of magnitude or even becomes numerically zero in portions of the integration domain. The new technique is closer to standard multi grid, but restriction and prolongation are based on the base-function approach from MSFV. Applications to the solution of the incompressible Navier-Stokes equations with the immersed-boundary technique are presented.

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CP5

A Second-Order, Three Level Finite Element Approximation of An Experimental Substrate-Inhibition Model

This paper is concerned with a second-order, three level piecewise linear finite element scheme for approximating the stationary (Turing) patterns of a well-known experimental substrate-inhibition reaction-diffusion system ('Thomas system'). A numerical analysis of the semi-discrete in time approximations leads to semi-discrete *a priori* bounds and an error estimate. We illustrate the numerical solutions of the fully-discrete finite element method by approximating the Turing patterns over a schematic mammal coat with fixed geometry at various scales.

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CP5

Approximation Capability Of A Bilinear Immersed Finite Element Space

We discuss a bilinear immersed finite element space for solving second order elliptic boundary value problems with discontinuous coefficients. This is a nonconforming finite element space and its partition can be independent of the interface. First we show some basic properties of this space. Then by using multi-variable Taylor expansion technique, we prove the optimal approximation capability of this space. Finally, we use numerical examples to demonstrate features of this IFE space.

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CP5

The Numerical Analysis of Singular Solutions to Partial Differential Equations

. Singularities often occur in solutions to partial differential equations; one of the important examples includes the formation of shock fronts in hyperbolic equations. In this talk, we present a new method for the numerical analysis of complex singularities in solutions to partial differential equations. In this method, we analyze the decay of Fourier coefficients using a numerical form fit to ascertain the nature of singularities in two and three-dimensional functions. As an example, we apply this method to analyze the complex singularities for the 2D inviscid Burger equations.

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CP5

Mixed Finite Element Methods for the Fully Nonlinear Monge-Ampre Equation Based on the Vanishing Moment

This talk is concerned with studying mixed finite element approximations of the viscosity solution to the Dirichlet problem for the fully nonlinear Monge-Ampère equation $det(D^2u^0) = f\,(>0)$ based on the vanishing moment . In this approach, the fully nonlinear Monge-Ampère equation is approximated by the fourth order quasilinear equation $-\epsilon\Delta^2u^\epsilon + detD^2u^\epsilon = f$. We develop a family of Hermann-Miyoshi type mixed finite element methods for approximating the solution u^ϵ and the moment tensor $\sigma^\epsilon := D^2u^\epsilon$.

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CP5

Adaptive Fem Based on Cvt and Superconvergence

In this article, a novel adaptive finite element method is presented, which is based upon Centroidal Voronoi tessellation (abbr. CVT) and superconvergent gradient recovery. Due to the nice mesh quality guaranteed by the construction of Centroidal Voronoi Delaunay Triangulation, asymptotically exact error estimation can always be obtained, which results in a convergent adaptation procedure. The Lloyd iteration is localized and adapted for local remeshing which is a key part of the mesh adaptation procedure. Various numerical examples for elliptic equations are presented to demonstrate the effectiveness of the proposed approach.

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CP6

Recent Progress in Modeling the Human Tear Film

We report on recent results in from our modeling efforts to better understand the dynamics of the human tear film. Lubrication theory is used to reduce the problem to a nonlinear one-dimensional partial differential equations governing the tear film thickness. The curvature of the (ellipsoidal) cornea is studied in a model problem that illustrates the influence of this aspect of the eye. Other progress will be discussed as available.

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CP6

Effective Numerical Resolution of Bidomain Equations for Action Potential Propagation in the Heart

We study the action potential propagation in the myocardial tissue using the Bidomain macroscopic model, coupled with models for the ionic cell currents (Rogers-McCulloch, Luo-Rudy). Since solving the Bidomain model is very expensive, we are investigating several methods to reduce its computational costs without loosing accuracy. We present a preconditioner for the Bidomain system based on the simplified Monodomain problem, tested on both 2D and 3D geometries. Adaptive modeling strategies are considered as well.

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CP6

Classification of Cerebral Aneurysms: the Role of Geometry and Haemodynamics of Internal Carotid Artery

We address morphological and fluid-mechanical features of Internal Carotid Artery (ICA) possibly related to cerebral aneurysms presence and rupture (a dramatic event). A classification is presented, based on functional data analysis of ICA radius and curvature extracted from clinical images. Computational fluid dynamics of blood flow in vessels belonging to different classes show relevant differences, being the risk of rupture potentially quite different among the classes. Classification could have therefore a significant predictive role.

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CP6

Computational Fluid Dynamics and Biochemics in Cerebral Focal Ischemia

This work concerns mathematical and numerical modeling of focal ischemia in tridimensional geometries. A major problem while treating focal ischemia is that pharmacological reperfusion of the brain could lead to hemorrhage. The proposed model includes a space dependent description of the blood dynamics considering the brain as a porous medium and a description of ionic disorder/tissue damage rate caused by a reduction in the flow rate (spreading depression). 3D numerical simulations are presented.

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CP6

Modeling Folding Patterns in the Human Brain

The human cerebral cortex is a highly folded surface. How these folds occur, and their significance, has fascinated scientists across a variety of disciplines. My research aims to

answer some of these questions by using a Turing reaction-diffusion system on a prolate spheroidal domain and see how domain size and shape play a key role in cortical patterning.

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CP6

Harmonic Analysis for Cognitive Vision Systems: Perisaccadic Mislocalization

In the conformal camera, image transformations are given by the group SL(2,C). The group Fourier transform is computable by FFT in complex-logarithmic coordinates. In neuroscience, these coordinates approximate the retinotopic mapping of the brain's visual pathway. Thus, it provides image representation that numerically integrates the head, eyes and visual cortex. Here we include the visual field and eyes saccadic movement and explain how the perisaccadic space compression can be approached numerically in our binocular system.

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CP7

An Analysis of Method of Fundamental Solutions for Neumann Problems of Laplace's Equation

Most of the existing analysis for the method of fundamental solutions deals with Dirichlet problems of Laplace's equation on disk domains. This paper is devoted to the analysis for the Neumann problems in bounded-simply connected domains, accompanied with the bounds of both errors and condition numbers. Numerical experiments are provided to support the analysis made.

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CP7

Stability Analysis of Method of Fundamental Solutions for Mixed Problems of Laplace's Equation

For the method of fundamental solutions, new approaches are proposed for deriving the growth asymptotes of condition number (Cond), and applied to solving Laplace's equation. The sharp bound of Cond is derived for disk domains, and for bounded simply-connected domains with mixed boundary conditions. Numerical results are reported to support the analysis made.

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CP7

Multiscale/multigrid Method for Finding a Full Eigenbasis of the Schrdinger Operator

Many applications involving differential operators require a knowledge of their many eigenfunctions. In this talk we will introduce a novel multigrid approach that, by employing a multiscale structure for eigenfunctions' approximation, allows calculating all eigenfunctions of the Schrödinger operator and performing many applications typical for eigenvalue problems in just $O(N \log N)$ operations, where N is the size of the discretized problem. We will conclude with numerical experiments and a discussion of the further extension of the approach.

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CP7

High Order Accurate Interpolation Schemes for Solutions of Elliptic Equations

We present a new class of highly accurate two and three dimensional interpolation schemes. These schemes were originally designed to be used in particle mesh calculations for calculating the field on a collection of charged particles, but can also be used for interpolating a broad class of other functions. In particular, our schemes work well for interpolating functions which satisfy Laplace's equation, and can also be used to accurately interpolation functions which satisfy other homogeneous elliptic differerential equations. This set of equations includes ones with discountinuous coefficients provided the discontinuities lie on straight lines. The schemes can also be used for interpolating other functions, although the results are less accurate.

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CP7

Variational Problems in Weighted Sobolev Spaces on Non-Smooth Domains

We study the Poisson problem $-\Delta u = f$ and Helmholtz problem $-\Delta u + \lambda u = f$ in bounded domains with angular corners in the plane and $u = 0$ on the boundary. On non-convex domains of this type, the solutions are in the Sobolev space H^1 but not in H^2 even though f may be very regular. We formulate these as variational problems in weighted Sobolev spaces and prove existence and uniqueness of solutions in what would be weighted counterparts of $H^2 \cap H_0^1$. The specific forms of our variational formulations are motivated by, and applied to, a finite element scheme for the time-dependent Navier-Stokes equations.

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CP7
Numerical Solutions of Boundary Inverse Problems for the Lapace Equation

Based on a boundary integral equations formulation, we present numerical solutions for two inverse problems for the Robin boundary value problem for the Laplacian: (1) the inverse problem of recovering the Robin coefficient from a boundary measurement of the solution on a portion of the domain boundary, and (2) the inverse problem of recovering part of the Robin boundary from multiple sets of partial boundary measurements.

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CP8
On the Discrete Adjoints of Adaptive Numerical Integration Algorithms

We investigate the behavior of adaptive time stepping algorithms under the reverse mode of automatic differentiation (AD). Reverse-mode differentiation of the time step controller and the error estimator in the forward method leads to spurious adjoint derivatives of the time steps. These perturbations make the resulting discrete adjoint models inconsistent with the adjoint ODE. To regain consistency, one has to cancel out the contributions of the non-physical derivatives in the discrete adjoint model. We demonstrate that the discrete adjoint models of one-step, explicit adaptive algorithms, such as the Runge-Kutta schemes, can be made consistent with their continuous analogs using simple code modifications. We extend the analysis to second order adjoint models derived through an extra forward-mode differentiation of the discrete adjoint code. Two numerical examples support the mathematical derivations.

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CP8
Verified Numerical Error Estimates for Non-Product Cubature by Kernel Methods

Sard kernels theorems offer important tools for discussing the errors of multivariate linear approximation problems. Through interval computation, they can be completely applied to numerical error estimation. The main task thereof is to evaluate the Sard error constants by root finding, which, however, is a nontrivial task. The numerical methods and difficulties for computing the error constants are to be discussed. As practical applications, numerical error bounds for non-product cubature are to be presented.

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CP8
Computing Highly Oscillating Integrals Using Euler-Longman-Lyness Summation

In this talk we demonstrate how Euler-Longman-Lyness summation may be used to compute highly oscillating (finite) integrals. The technique may be applied to problems with nonlinear monotonic phase functions allowing stationary points at the interval endpoints only. The algorithm developed is making use of the fact that the circular functions are periodic and combines zero-finding codes with adaptive quadrature algorithms to compute some of the terms in a finite series. Examples demonstrate that only information close to the interval endpoints is used in the results. The effect of having stationary endpoints is that information further away from the endpoints is needed in order to compute good estimates.

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CP8
Numerical Conformal Mappings of Multiply Connected Domains by the Charge Simulation Method

The basic idea of the charge simulation method is to approximate the harmonic functions with boundary conditions by a linear combination of logarithmic potentials. We extended the method by use of complex logarithmic potentials to approximate analytic functions as the conformal mapping functions. By our method, conformal maps from bounded and unbounded domains of arbitrary order of connections, which have smooth boundary curves, onto various types of canonical domains including all the types of Nehari's canonical slit domains are available.

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CP8
Improved Contour Integral Methods for Parabolic PDEs

One way of computing the matrix exponential that arises in semi-discrete parabolic PDEs is via the Dunford-Cauchy integral formula. The integral is approximated by the trapezoidal rule on a Hankel contour defined by a suitable change of variables. In a recent paper by the speaker

and LN Trefethen [Math. Comp., Vol. 76, pp. 1341–1356 (2007)] two widely used contours were analyzed. Estimates for the optimal parameters that define these contours were proposed. In this talk, that analysis is extended in two directions. First, the effect of roundoff error is now included in the error model. Second, we extend the results to the case of a model convection-diffusion equation, where a large convective term causes the matrix to be highly non-normal.

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CP8

A Second Order Algorithm for Curvature Calculation with Meshed Hypersurface

We propose a second order curvature calculation for curves and surfaces via polynomial and least square fittings. The algorithm is second order in space and is coupled with second order in time when implemented in front tracking. This method is more efficient, accurate and robust to noise than direct interpolation. Both normal and curvature computed by this method is sufficiently smooth even if the positions of vertices are not.

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CP9

Stability and Dispersion Analysis of a Finite Element Method for Maxwell's Equations in Dispersive Media

In this talk we discuss the stability properties and the phase error of a finite element scheme for Maxwell's equations coupled with a Debye or Lorentz polarization model for modeling wave propagation in dispersive media. We present numerical simulations which validate our analytical results and determine a practical guideline for the choice of discretization parameters. We also compare this method with finite difference methods that have been analyzed in the literature.

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CP9

The Method of Fundamental Solutions for Helmholtz Equation

Helmholtz equation is an important equation in engineering with many applications, e.g. electromagnetism. We plan to use two major boundary methods, method of fundamental solution and Trefftz method, to compute its numerical solution. For the former, we try Bessels functions of first kind and second kind as basis functions respectively. The mathematical equivalence of both methods is uncovered. We will also compare the efficiency of both methods. Finally we have some theorems of error and stability analysis for the method of fundamental solution.

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CP9

Solving MHD Equations by a Local Characteristic Based Upwind Scheme

We present an appropriate spectral decomposition in local wavefields of the ideal magnetohydrodynamic (MHD) equations that allows determining the non convexity of the nonlinear characteristic fields. We propose an upwind scheme based on the local characteristic decomposition that mimics the entropy satisfying Lax-Friedrichs scheme applied to non convex scalar conservation laws. High order versions of the scheme are tested through a set of one and two dimensional MHD numerical examples.

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CP9

Dynamics of Light Channel Switching in Nonlinear Optical Media

The dynamics of two light beams interacting at an interface separating tow nonlinear optical media is studied numerically and analytically. The trapped beam at the interface acts as a power controllable switch to reflect or transmit the incident beam at the interface. This results can be used to develop a device in signal switching.

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CP9

Efficient Band Edge State Calculation in Electronic Nano Structures

This talk compares techniques for the computation of band edge states of electronic nano structures. The mathematical formulation as a sparse Hermitian interior eigenvalue problem poses unique challenges to existing algorithms which are discussed together with efficient ways to address them.

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CP9

4th Order Embedded Boundary Method for the Maxwell Equations

A fourth order embedded boundary method for the Maxwell equations in geometrically complex domain has been developed. The fourth order accuracy is achieved by building of high order mappings between cell averages and point values for the magnetic field in cut cells, and high order polynomial representations of the electric field along the grid lines. The time integration is based on Yoshida's method of building symplectic higher order schemes from lower order ones. The motivation is to improve solutions in geometrically complex domains and avoid numerical difficulties typical for unstructured finite element schemes for the simulations of electromagnetic waves coupled with charges particles.

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CP10

The Change in Electric Potential Due to Lightning

The change in the electric potential due to lightning is evaluated. The potential along the lightning channel is a constant which is the projection of the pre-flash potential along a piecewise harmonic eigenfunction which is constant along the lightning channel. The change in the potential outside the lightning channel is a harmonic function whose boundary conditions are expressed in terms of the pre-flash potential and the post-flash potential along the lightning channel. The expression for the lightning induced electric potential change is derived both for the continuous equations, and for a spatially discretized formulation of the continuous equations.

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CP10

Analysis of Lightning Charge Transport

Techniques are developed for inverting measurements for the electric field obtained by a balloon-borne sonde (or Esonde) to estimate the charge transport associated with lightning. The techniques are applied to a thunderstorm occurring on 18 August, 2004, near Langmuir Laboratory in New Mexico. This analysis leads to a picture for how charge flows in the 30 km region observed by the balloon.

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CP10

Modeling Fractures as Interfaces: Nonconforming Grids and a Posteriori Estimates

Numerical modeling for flow in porous media is complicated by the presence of fractures in the medium. These fractures can act as privileged channels for flow or they can act as barriers, yet they are difficult to include in a numerical model because their width is very small in comparison to the size of the domain. Small networks of interconnected fractures are often taken into account by homogenization, but this method is not appropriate for larger, individual fractures. One method that has been proposed for such larger fractures is to treat them as surfaces or interfaces. In this talk we are concerned with this latter type of model and in particular with adaptive grid refinement in and around the fractures. We consider the issue of nonconforming grids and we use a posteriori error estimates for refining the grid.

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CP10

Atmospheric Retention of Man-made Carbon Dioxide Emissions

For 1850-2000, atmospheric CO_2 concentration $c(t)$ can be related to man-made CO_2 emissions $P(t)$ by a linear reqression model $\mathbf{c(t)} = \mathbf{P(t}, \tau)\mathbf{q}(\tau) + \epsilon(\mathbf{t})$ where the $q(\tau)$ are unknown retention fractions. Gaps in the $c(t)$ record make the system underdetermined but the constraints $0 \leq q(\tau) \leq 1$ make estimation tractable. O'Leary's BRAKET-LS algorithm is used to compute confidence intervals for $q(t)$ averages on suitably chosen time subintervals and show that a statistically significant increase in $q(t)$ occurred in ~ 1900.

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CP10

Particle Filtering with An HMC/PMMC Step and an Application to a Bimodal Ocean Current Model

In this presentation I will introduce a recursive Monte Carlo algorithm designed to filter high dimensional stochastic dynamical systems with complicated non-linear and non-Gaussian effects. The method incorporates parallel marginalization and hybrid Monte Carlo to improve the samples generated by standard particle filters. As a

validation the algorithm is tested on a 2516 dimensional, bimodal, stochastic model motivated by the Kuroshio current that runs along the Japanese coast.

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CP10

Elliptic Equations in a Highly Heterogeneous Porous Medium

Elliptic equations in a highly heterogeneous porous medium arise from many problems, for example, in the study of flow in fractured media or the study of stress in composite media and so on. The medium basically consists of a connected fractured region with high permeability and a disconnected matrix block region with low permeability. Let ϵ denote the size ratio of one matrix block to the whole domain. In the fractured sub-region, Hölder and Lipschitz norms of the elliptic solutions are bounded uniformly in ϵ as well as convergence rate of the solutions in L^∞ norm can be estimated. By means of these results, we are able to explain why a microscopic model, which describes the effects of turbulent mechanical mixing of non-stationary, incompressible, two-component, miscible displacement in fractured media converges to a dual-porosity model as ϵ tends to 0.

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CP11

A Subspace Minimization Method for the Trust-Region Step

We consider methods for large-scale unconstrained optimization based on finding an approximate solution of a quadratically constrained trust-region subproblem. The solver is based on sequential subspace minimization with a modified barrier "accelerator" direction in the subspace basis. The method is able to find solutions of the subproblem to any prescribed accuracy. Numerical results will be presented. This is joint work with Philip Gill and Joshua Griffin.

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CP11

Efficient Best-Approximation of Tensor Sums and Applications

If an algorithm in one-dimension is extended to dimension d, its computational cost grows to the power of d in almost every case. Tensor sums (TS) are promising objects for multi-dimensional problems. Linear algebra operations can be performed in this representation using only d times one-dimensional operations. In iterative methods with tensor sums, it is important to solve the following problem. For a given tensor sum $A = \sum_{i=1}^{R} \otimes_{\mu=1}^{d} A_{i\mu} \in \mathrm{TS}(R)$ and $\varepsilon \in R_+$, find $X^* = \sum_{i=1}^{r_\varepsilon} \otimes_{\mu=1}^{d} X^*_{i\mu} \in \mathrm{TS}(r_\varepsilon)$ such that:

$$\begin{aligned} \|A - X^*\| &\leq \varepsilon, \\ \|A - X^*\| &= \min_{X \in \mathrm{TS}_c(r_\varepsilon)} \|A - X\|. \end{aligned}$$

We will introduce a new trust region Newton method that solves this approximation problem in arbitrary tensor product pre-Hilbert spaces. Finally we will present numerical results in high dimensions.

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CP11

A Solver Interface for Stochastic Programming Problems

Stochastic programming problems can often be represented as large-scale structured mathematical programs and solved using specialized algorithms. These require specialized information, such as time stages and distributions. As new model types emerge, for instance, nonlinear objectives and constraints, stochastic problem dimensions, nonuniform time horizons, etc., the well-known SMPS format is no longer adequate to communicate these peoblems to a solver. This talk describes a proposal based on an XML schema. It supports deterministic programs as well as scenario and distribution-based stochastic programs, robust optimization, chance constraints, etc. Examples are used to ilustrate the use of the schema. The implementation of a parser and solver interfaces are described as well.

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CP11

Derivative-Free Optimization Methods for the Calibration of Groundwater Bioremediation Models and Watershed Models

We consider two computationally expensive environmental optimization problems, namely, the calibration of a watershed model and the calibration of a PDE-based groundwater bioremediation model of chlorinated ethenes. We solve these problems using different types of derivative-free optimization methods, including radial basis function algorithms, derivative-free trust-region methods, pattern search, and heuristic optimization techniques. The results indicate generally good performance for methods that utilize some form of approximation model of the calibration objective function.

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CP11

A Generalized Primal-Dual Augmented Lagrangian

We consider methods for large-scale nonlinear non-convex optimization. A class of primal-dual augmented Lagrangian active-set methods is proposed in which optimization occurs simultaneously with respect to both the primal and the dual variables. This class includes second-derivative sequential quadratic programming methods with guaranteed convergence.

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CP11

Efficient Grassmann-Quasi-Newton Algorithms for Best Multilinear Rank Approximation of Tensors

In this talk we will present state of the art algorithms for solving the best multilinear rank approximation problem of tensors. We exploit the fact that the problem may be viewed as an optimization problem over a product of Grassmann manifolds and construct the algorithms using BFGS and limited memory BFGS updates specifically adapted for Grassmannians. We will present experimental results and compare the performance of the different algorithms in terms of computational efficiency and memory usage. Tensor approximation problems occur in various applications involving multidimensional data, signal processing and pattern classification.

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CP12

Turbulent Flow and Heat Transfer Characteristics in U-Tubes: A Numerical Study

Using the standard k-e model, 3-dimensional turbulent flow and heat transfer characteristics in U-Tubes were investigated. Uncertainty was approximated using experimental correlations and grid independence. Increasing the Dean number was shown to intensify a secondary flow in the curved section. The overall Nusselt number for the tube was found to decrease substantially relative to straight tubes, while the overall skin friction coefficient remained practically unaffected. Local skin friction coefficient, Nusselt number, and wall temperature along the tube wall are presented.

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CP12

Theoretical Analysis of Generalized Level Crossings of Multiscale Fields with Applications to Turbulence

We theoretically analyze a new approach which provides a useful tool for studies of generalized level crossings in multiscale phenomena. The method enables the definition of generalized level crossing scales and analysis of their probability density function, by generalizing the one-dimensional concept of level crossing scale to multidimensional fields in terms of the shortest distance from random locations, within a reference region, to the nearest level crossings. Computations and experiments are also presented with applications to turbulence.

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CP12

Turbulence Modeling for Vortex Dominated Flows

Large-eddy simulation (LES) has become an attractive approach for the numerical simulation of vortex dominated flows while the use of unsteady Reynolds-averaged Navier-Stokes (URANS) is still subject of debate. Although extensive research, regarding the numerical simulation of turbulent flows, has been carried out, there are still many fundamental questions that have to be addressed. The goal of the present investigation is to highlight the fundamental differences between LES and RANS turbulence models, for vortex dominated flows.

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CP12

Space Map Hierarchy for Particle Control in Turbulent Flows

The simulation and optimal control of particles suspended in turbulent flows is of great interest for glass wool production processes. In this work, we present a model and a space map approach for the particle control in turbulent flows. The used space map hierarchy is based on the combination of a k-epsilon turbulence model for high Reynolds-number flow with several DNS-simulations of smaller Reynolds-number flows on coarser grids. The numerical results are very promising and provide an answer to the questions of stochastic control.

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CP12

Numerical Analysis of Turbulence Models

This talk addresses the mathematical approach in which we bridge some gap between theory and computations. Accurate, efficient and reliable simulation of turbulent flows is an essential difficulty in many current industrial applications. To that end, I will present a numerical study of a family of high accuracy turbulence models, the Leray-deconvolution family. Numerical experiments in 3d which confirm the convergence theory and numerical experiments for the 2d step problem will be presented.

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CP13

A Moving Mesh Method for Scale-Invariant PDEs

Self-similar solutions of scale-invariant nonlinear partial differential equations play an important role in understanding the behaviour of physical phenomena. Such solutions possess a time-invariant integral, as do their L_2 projections. Conversely, time-invariance of the integral implies that a self-similar solution is evolved exactly in time (a symmetry preserving property of the invariance). The invariance can be used as the basis of a velocity-based multidimensional moving mesh method which can approximate simple intermediate asymptotics.

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CP13

Solving Time-Dependent Pdes Using the Material Point Method, Accuracy and Error

The Material Point Method (MPM) developed by Sulsky and colleagues is currently being used to solve many challenging problems involving large deformations and/or fragementations with some success. In order to understand the properties of this method an analysis of the considerable computational properties of MPM is undertaken in the context of a model problem from gas dynamics. The MPM method in the form used here is shown to have first order accuracy using analysis related to Monte Carlo Methods

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CP13

Counter Examples to the Sonic and Detachment Criteria

Mach and von Neumann have asked when the reflection of shock waves in compressible fluids from solid walls is "regular" (RR) rather than "Mach type". Numerics and experiments have not settled the problem unambiguously. Two criteria, sonic and detachment, compete in predicting the right transition point. We give counterexamples to both criteria. In two separate reflection problems, one in self-similar potential flow and one in steady full Euler flow, we shows that solutions with transonic reflected shock exist and are stable under parameter and boundary perturbation. This demonstrates that the sonic criterion is not correct. Moreover we present counterexamples to the detachment criterion in a special but significant part of the parameter set.

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CP13

Convergence Analysis of a Space-Time Discontinuous Galerkin Method for Scalar Conservation Laws

In 2004, Palaniappan, Haber, and Jerrard introduced a new promising space-time discontinuous Galerkin (STDG) method for scalar conservation laws. We obtained L^1 estimates and entropy inequalities of the approximate solutions of this method, from which we proved the convergence of the approximate solutions to the entropy sotuion with the rate of convergence at least $h^{\frac{1}{4}}$ in L^1 norm, by applying the results on Kruzkov's estimates done by Bouchut and Perthame.

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CP13

Integral Equation Methods for Incompressible

Fluid Dynamics

We present new integral equation formulations for the incompressible Navier-Stokes equations. In two dimensions, this involves working with the stream-function formulation. After a suitable temporal discretization, a modified biharmonic equation remains. This equation is recast as a well-conditioned integral equation. When coupled with modern fast algorithms (such as the Fast Multipole Method), these integral equation methods will be highly accurate and efficient. As shown in previous work for the Stokes equations (Greengard, Kropinski, Mayo 1996), we anticipate being able to solve large-scale problems with highly complex geometry.

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CP13
The Immersed Interface Method for Simulating Prescribed Motion of Rigid Objects in a Flow

A solid boundary immersed in a fluid can be formulated as a singular force in the Navier-Stokes equations. Two problems arise regarding this formulation. One is how to calculate the singular force. The other is how to treat the force singularity. The latter is solved in the immersed interface method with second-order accuracy and the sharp fluid-solid interface by incorporating singularity-induced flow jump conditions into discretization schemes. This talk focues on the former problem. In particular, I will present an explicit approach for computing the singular force to enforce prescribed motion of a rigid boundary in an incompressible viscous flow. This approach eliminates ad hoc penalty models for rigid boundaries and associated stiffness, which gives it numerical stability at relatively high Reynolds numbers. Simulations of circular Couette flow, flow past a cylinder, and flow around flappers will be shown to test the accuracy, stability, and efficiency of this approach.

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CP14
An Interlaced Time Stepping Method for Stiff Systems of Stochastic Differential Equations

For stiff stochastic systems, the fluctuations off the slow manifold might not be negligible in size, and an implicit scheme will dampen all these fluctuations and therefore will fail in computing the variance correctly. We present a time-stepping strategy, by interlacing an implicit Euler time step with a sequence of optimal number of explicit Euler time steps, such that the computed asymptotic variance is the closest to the correct variance of the stationary distribution.

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CP14
Traffic Flow Model of the Internet

We derive a model of packet traffic which replicates key aspects of the internet, with results closely portraying the flow. We develop a node/link network model of traffic flow, emphasizing packet queuing and the flow of packets from spatial point to spatial point. The continuum aspect of the model will lead to fluid-like equations that will be used to predict changes in global flow patterns and optimal paths in the network.

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CP14
Stability of Fronts in a Gasless Combustion Model

I will discuss stability of fronts in a model describing gasless combustion of one-dimensional solid fuels. Carefully chosen exponential weights stabilize the spectrum of the front, but neither the linear nor the nonlinear stability cannot be simply inferred from the spectral stability. A more subtle analysis is necessary to show that the front is orbitally stable in the weighted norm. Co-authors: Y. Latushkin, S. Schecter, and A. J. De Souza.

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CP14
Traveling Wave for a Thin Liquid Film with Surfactant on An Inclined Plane

We show the existence of traveling wave solutions via geometric singular perturbation theory for a lubrication model for a surfactant-driven flow of a thin liquid film down an inclined plane. We construct the solutions in certain singular limits, and then we extend the parameter regimes where the solutions exist.

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CP14
On the Nearest Non-Minimal Systems Reducible to Prespecified Order

Given a dynamical system of order n (dimension of state state space) we investigate the distance to the nearest system that is equivalent to a system of order $r < n$. This measure is closely related to the distance to the nearest system whose reachable subspace is at most of dimension r for which we provide a singular value optimization characterization. The characterization is inspired by Malyshev's formula for the distance of a matrix to having a multiple eigenvalue.

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CP14

Asymptotic Dynamics of Attractive-Repulsive Swarms

A challenge in swarm modeling is to choose a description of social interactions that produces qualitatively correct macroscopic behavior. We study the 1-d swarming model $\rho_t + [\rho(f_s * \rho)]_x = 0$. We determine conditions on the (general) social interaction kernel f_s for the population density profile ρ to asymptotically spread, contract, or reach steady state. We further analyze the spreading case, for which ρ obeys porous medium dynamics, and the contracting case, for which $\int \rho$ obeys Burgers-like dynamics.

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CP15

Microlocal Corrections and Strong Limits in Homogenization and Semiclassical Problems

Microlocal defect measures and Wigner measures have been used in the study of semiclassical and homogenization limits. Usually these limits are weak; in addition 'ε-dependent corrections' are often hard to construct. A regularized microlocal transform is used, allowing for the formulation of convergence results in Banach spaces (related to Gelfand-Shilov type spaces), and the formulation of a hierarchy of rigorous asymptotic approximations. Case studies and numerical applications are also examined to illustrate further the result.

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CP15

Using Optimal Time Step Selection to Boost the Accuracy of Finite Difference Methods for Time Dependent PDEs

This talk presents a novel technique based on optimal time step selection that transforms low-order finite difference schemes into high-order numerical methods for time dependent PDEs. For example, optimal time step selection can achieve high-order accuracy using simple schemes based on forward Euler time integration and low-order stencils for spatial derivatives. We demonstrate the utility of optimal time step selection on several classical PDEs in one and two space dimensions (on both regular and irregular domains) and explain the observed orders of convergence through straightforward numerical analysis arguments.

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CP15

Modeling and Simulation of Grain Growth

Simulation is becoming increasingly important in the study of grain growth, because a central problem in materials science is the understanding and control of microstructures in polycristalline materials. We present a variational approach to mesoscale simulations of large networks of grains. The evolution is governed by Mullins Equations of curvature driven growth. We show 2-dimensional simulation results for a curvature driven model as well as for a vertex model, which agree well with experimental results.

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CP15

Micromechanics of Quasi-1D Compaction Waves

A combined finite and discrete element method is used to examine the micromechanics of piston driven weak quasi-1D compaction waves within a 2D particle system. The method combines conservation principles with an elastic-viscoplastic and friction constitutive theory to predict velocity, strain, and stress fields within particles resulting from both particle-piston and particle-particle interactions. Emphasis is placed on characterizing the temporal and spatial partitioning of particle energy within compaction wave structures that result from low speed piston impact (100-300 m/s) and analyzing their dependence on piston speed, particle size distribution, and particle material properties.

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CP15

Two-Dimensional Convection Diffusion Past a Circle

We consider the concentration of some substance in $\mathbf{R}^2$ exterior to the unit circle. The substance diffuses in the plane and is convected to the right by a uniform field. The concentration satisfies a linear elliptic PDE. We explicitly solve this problem and evaluate the solution in the asymptotic limit where convection dominates diffusion (i.e., the Peclet number is large). We also apply singular perturbation methods to achieve the same results.

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CP15

Fast Marching Methods for Adaptive Non-Graded

Cartesian Grids

We present a level set scheme utilizing fast-marching methods for non-graded Cartesian grids with adaptive remeshing. We use quadtree data structures and an automated meshing algorithm to describe general shapes in two dimensions. The fast-marching method is adapted for use with the non-graded Cartesian grid and utilized for both level set re-distancing and front advancement. The use of volume-of-fluid mass correction will also be discussed.

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CP16

Random Numerical Discretizations

The question of gridpoint selection is a challenging problem in many areas of numerical analysis. In this talk, I will present out methodology for using a low order sampling scheme to construct higher order solutions to a Poisson equation. The core idea involves carefully formulating an inverse problem to identify a probability measure assigning a high probability to favorable grid point locations (similar to importance sampling in Monte Carlo methods). I will provide results of the application of this technique as well preliminary results on generalizing the technique to higher dimensions.

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CP16

Computing Multivalued Solutions of Pressureless Gas Dynamics by Deterministic Particle Methods

We consider one- and two-dimensional pressureless gas dynamics equations. These equations arise in different applications and, in particular, in semiclassical approximations of oscillating solutions of the Schrödinger equation with the high frequency initial data. In this case, multivalued solutions of the pressureless gas dynamics equations are physically relevant. We compute these multialued solutions using a deterministic particle method. Point values of the computed solutions are recovered from their particle approximations using different smoothing procedures. We study several recovery strategies and demonstrate ability of the particle method to achieve a high resolution on a number of numerical examples.

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CP16

A 3D PIC-DSMC Method for Simulation of Low Temperature Non-Continuum Plasmas

A production 3D hybrid PIC-DSMC simulation tool has been developed for the simulation of low temperature non-continuum plasma phenomena. We have incorporated unstructured meshes, dynamic load balancing, per-particle weightings, and chemistry all in one code. A novel hierarchical evaluation infrastructure has been implemented to minimize the cost of introducing new computational kernels for algorithmic or post-processing purposes. Scaling studies and examples will be presented.

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CP16

Adaptive Multigrid Phase-Field Simulations of Rapid Solidification

This talk will describe our recent advances in numerical simulation using phase-field models based upon a fully-implicit, adaptive, multigrid implementation. Initial work in two dimensions has led to the ability to solve coupled thermal-solute models for dilute alloy solidification using physically realistic parameters for the first time. These results will be enhanced with those from our current project which is extending this work to three-dimensional models using parallel computing architectures.

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CP16

Lagrangian Particle Method for Electrostatic Plasmas

In the Eulerian formulation of an electrostatic plasma, the electron pdf satisfies the Vlasov-Poisson equations. Here we employ an alternative Lagrangian formulation in terms of the electron flow map. This leads to a particle method in which the self-consistent electric field is a sum of particle-particle interactions. The numerical method uses regularization, adaptive particle insertion, and a hierarchical

treecode. Simulations of particle transport in electron beams are presented.

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CP16

A Comparison of the Common Semi-Implicit Time Stepping Schemes in a Spectral Method Navier-Stokes Solver

The semi-implicit time stepping schemes: Adams-Bashforth/Backward-Differencing (ABBDI2), Adams-Bashforth/Crank-Nicolson (ABCN), Modified ABCN (MABCN) and Leap frog were implemented in a spectral methods based Navier-Stokes solver. The solver utilizes FFT to handle Fourier expansions in the two directions and Chebychev polynomial expansion in the third direction. The solver was used for obtaining time dependent velocity and temperature fields for a natural convection in an inclined channel problem. Among these four most common semi-implicit time stepping methods, MABCN is determined as the most stable one. For this application, we have seen only minor stability improvements when MABCN or ABBDI2 was used instead of ABCN. The improvements were not enough to allow for a time step size reduction but they were enough to decrease initial oscillations on the global solution. The comparative results and the comparisons with the previous literature are presented in terms of dimensionless groups.

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CP17

Cascades and K-Cores on Complex Networks

Network models underlie many complex systems, e.g. Internet, WWW, gene-regulatory networks, etc. Here an analytical approach to determining the mean avalanche size in a broad class of dynamical models on random networks is introduced. Previous results on percolation transitions and epidemic sizes are shown to be special cases of the method. Examples giving the rate of spread of innovations in a community-structured network and the size of k-cores in correlated networks agree with numerical simulations.

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CP17

An Infinite-Buffers Tandem Queueing System

An infinite-buffers tandem queueing system featuring feedback and task-splitting is considered. An algorithm is given to solve the functional equation driven from the system of differential difference equations of the stationary queue length process using Hilbert Problem approach. The numerical challenges of the problem will be discussed.

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CP17

Joint Determination of Optimal Price and Procurement Quantity for An Item on Sale When the Demand Is Stochastic

We consider the joint replenishment decision problem when an item is on sale with temporary price discount and the demand follows some stochastic process. The considered cost includes: procurement cost, inventory carrying costs for both the periods of sale event and afterwards, and the cost of lost sale due to shortage. Our decision problem is to jointly determine the optimal sale price and the replenishment quantity prior to the sale event so that the expected profit is maximized. The expected profit model is derived and analyzed. Under some mild conditions, the concavity of the expected profit function is established. An efficient search procedure is developed to find the optimal price and the procurement quantity. Computational studies are reported to illustrate the solution procedure; and some numerical results are summarized.

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CP17

The Probability Distribution of the Occupied Spaces of a Processor Sharing Storage Allocation Model

We consider a storage model with m primary holding spaces, infinitely many secondary ones, and a processor sharing server that services the stored items. All spaces are ranked and numbered, and a new customer occupies the lowest ranked space. We study the number of occupied spaces in this model, obtaining exact solutions for m=1 and m=2, and asymptotic ones for general (possibly large) m.

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CP17

Little's Formula for Cooperative Groups

It is one of the major challenges to explain cooperative behavior. The individual reward in cooperative group depends how we share the rewards in the group. Thus, the group size dynamics in a cooperative group and reward allocation rule seems essential to evaluate cooperative groups. We apply a sample-path based analysis called an extension of Little's formula to general cooperative group. We show that the expected reward is insensitive to the specific reward-allocation rule and probabilistic structure of group dynamics, and the simple productivity condition guarantees the expected reward to be larger than the average contribution. As an example, we take social queues to see the insensitivity result in detail.

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CP17

Asymptotic Theory of Sequential Change Detection and Identification

Suppose the distribution of a sequence of i.i.d. random variables changes suddenly at some unobservable time to one of finitely many distinct alternatives, then one needs to detect and identify the change at the earliest. We propose a sequential decision strategy that triggers an alarm when the posterior probability of a certain type of change exceeds some threshold, and show its asymptotic optimality under the Bayesian and the fixed-error formulations.

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CP17

Asymptotic Expansions For The Sojourn Time Distribution In Processor Sharing Queue

We consider $M/M/1$ and $M/G/1$ queues with a processor sharing (PS) server. We obtain the conditional sojourn time distribution, conditioned on the customer's service requirement, as well as the unconditional distribution, in various asymptotic limits. These include large time and/or large service request, and heavy traffic, where the arrival rate is only slightly less than the service rate.

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CP18

Dealing with Stiffness in Low-Mach Number Flows

In low-Mach number flows, the disparity of time scales between acoustic and convective motions introduce numerical challenges. A natural idea is therefore to separate the acoustic modes from the rest of the solution and to treat them implicitly, while the advective motions are treated explicitly or semi-implicitly. In this talk, we present a numerical allspeed algorithm that respects low-Mach number asymptotics but is suitable for any Mach number, and discuss benchmark results. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.LLNL-ABS-400392.

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CP18

Fast Explicit Operator Splitting Method for the Model of Propagation of Passive Pollutant in a Random Stirring Flow Field

Propagation of passive pollutants can be modeled by convection-diffusion equations. Such models arise in a variety of engineering and ecological applications, as well as in geophysical research. The pollutant diffuses while being transported by the governing flow, which leads to the stirring effect. This is the most mathematically interesting and challenging phenomenon, especially in the case when the stirring flow field is random. Development of reliable numerical methods for pollutant propagation models is crucial for understanding their properties—both physical and mathematical ones. I will present a fast explicit operator splitting method for these models with both deterministic and random velocity fields. The proposed method is successfully tested on a number of two-dimensional numerical examples.

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CP18

Smoothed Profile Method for Particulate Flows: Error Analysis and Simulations

We re-formulate and analyze a new method for particulate flows, the "Smoothed Profile" method (SPM), proposed by Y. Nakayama and R. Yamamoto (Phys. Rev. E. 71, 036707, 2005). The particles are represented by smoothed profiles, to construct a smooth body force added into the Navier-Stokes equations. While the original method employs a fully-explicit time-integration scheme we develop a high-order semi-implicit splitting scheme. We analyze the modeling error of SPM and show its dependence on the interface thickness of the smoothed profile and the time step size. Subsequently we extend the application of SPM to problems including shear flow past complex shaped parti-

cles and high Reynolds number cylinder flow.

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CP18

Stokes Flow Study by Fluid Particle Model with Single Particle

we developed a new form of Fluid Particle Model(FPM) which is a generalized dissipative particle dynamics(DPD) model, but including both linear and angular momentum so that we can investigate both translational and rotational motions of a single particle which was regarded as a sphere without internal structure, in different cases of unbounded or bounded low Reynolds number stokes flow at mesoscale level. All the simulation results agreed with the analytical results very well.

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CP18

A Spectrally Accurate Boundary Integral Method for Two-Dimensional Stokes Flows

A new numerical method is presented for interface dynamics in two-dimensional Stokes flows. It is based on the boundary integral formulation of the problem. The singular behavior of the integrands appeared in the boundary integral equations is analyzed and the equations are solved by Nystrom method. The method is spectrally accurate in space. The evolution equation is formulated in a theta-arclength coordinates and solved by Runge-Kutta method of second order. Several numerical examples are provided to verify theoretical prediction.

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CP18

Modeling and Numerical Simulation of Multiphase Flows

An energetic variational phase field model is proposed and used to study the pinch off phenomena of liquid filament. An efficient and accurate numerical scheme is presented and implemented.

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CP18

The Framework of k-Harmonically Analytic Functions for Three-Dimensional Stokes Flow Problems

The problems of 3-D Stokes flows due to the axially symmetric and asymmetric motions of solid bodies of revolution have been reduced to boundary-value problems for k-harmonically analytic functions, and the resisting force and torque exerted on bodies in corresponding motions have been expressed in terms of k-harmonically analytic functions. For domains, in which Laplace's equation admits separation of variables, the boundary-value problems can be solved in closed form based on representations of k-harmonically analytic functions in corresponding curvilinear coordinates. This approach has been demonstrated for solid sphere, prolate and oblate spheroids. As the second approach, the boundary-value problems have been reduced to integral equations based on the derived Cauchy formula for k-harmonically analytic functions and, as an illustration, have been solved for solid bi-spheroids and torus of elliptical cross section for various values of a geometrical parameter.

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CP19

A Partial Solution of the Aizerman Problem for Second-Order Systems with Delays

The paper considers the problem described by Rasvan [Rasvan, V. "Delay-Inepensdent and Delay-Dependent Aizerman Problem" in: Unsolved Problems in Mathematical Systems and Control Theory, V.D. Blondel and A. Megretski, eds., Princeton University Press, Princeton, NJ., 2004.] for second-order systems. The results are as follows: 1) For systems with a single delay not involving the second derivative, the Aizerman hypothesis is true. 2) For systems with multiple delays, not involving derivatives, a delay-dependent class of systems is identified, for which the Aizerman hypothesis is true. The proof of the results relies on the Popov's frequency-domain absolute stability criterion and on the Zhivotovsky's [El'sgol'ts, L.E. and Norkin, S.B. Introduction to the theory and applications of differential equations with deviating arguments, Academic Press, 1973.] absolute stability criterion for linear systems.

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CP19

Estimating the Fundamental Matrix of a Linear Delay Differential Equation

The monodromy operator of a linear delay differential equation with periodic coefficients is formulated as an integral operator. The kernel of this operator includes a factor formed from the fundamental solution of the linear delay differential equation. Although the properties of the fundamental solutions are known, in general there is no closed form for the fundamental solution. This talk describes a collocation procedure to approximate the fundamental solution before the integral operator is discretized.

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CP19

Reduction of Amplitude Equations by the Renormalization Group Approach

I will talk about the fundamental underlying structure of the Renormalization Group (RG) approach as it applies to the solution of differential equation involving multiple scales. The amplitude equation derived through the elimination of secular terms arising from a naive perturbation expansion of the solution to these equations, by the RG approach (Chen, Goldenfeld and Oono Phys. Rev. E **54** (1),1996) is reduced to an algebraic equation which is expressed in terms of the *Thiele semi-invariants or cumulants* of the eliminant sequence $\{Z_i\}_{i=1}^{\infty}$. I will illustrate its use through the solution of both linear and non-linear perturbation problems and recover certain results as special cases. The fundamental structure that emerges from the application of the RG approach is not the amplitude equation but the aforementioned algebraic equation. Reference: E.Kirkinis 'Reduction of Amplitude Equations by the Renormalization Group approach', Phy. Rev. E 77 (1) 011105 (2008)

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CP19

Efficient Symplectic-Energy-Momentum Integration of Hamiltonian Systems

A symplectic-energy-momentum integrator is a symplectic integrator which exactly conserves energy and momentum. Symplecticness implies the integrator can be derived from a discrete variational principle. The discrete variational principle gives the integrator coordinate invariant properties. The implicit equations of a symplectic-energy-momentum integrator are generally not easily solved, especially when the time step is small. An inefficient, nested iteration scheme is typically used to solve the nonlinear equations. We describe a new, more efficient, iteration which avoids nested iterations. We present simulation results for the nonlinear pendulum and Kepler's one body problem.

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CP19

Global Error Estimation for Odes and Method-of-Lines Pdes Using Adjoint Method and Defect Estimates

Global error estimation for initial value odes and method of lines pdes is considered by using adjoint-equation and defect estimates. The quality of defect estimates is shown to play a major role in the reliability of the global error estimates.

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CP20

Document Clustering on the Latent Projections

Data visualization (DV) allows identifying features and structure that may describe data. When DV is applied to text documents, it also let the analyst to observe sparseness in and between groups of documents, permitting to detect text similarity. In this work, a document clustering procedure is proposed based on the projections obtained for the latent variables in a modified version of the Generative Topographic Mapping (GTM) algorithm. The procedure is derived observing the latent variables structure when a Multinomial or Zero-Inflated Poisson model is implemented on GTM. An algorithm to detect class separation is derived consisting of three parts: first a group identification is realized, then a pair of groups are selected and the corresponding data are projected again on the trained GTM for visualization and a class overlapping identification is performed at last. An automatic document classification system is obtained, and a word analysis for groups, subgroups and overlapping class documents is presented, with a graphic representation of the data classes. Some structures on every classes are also discovered.

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CP20

Numerical Library Reusability for Large Scale Distributed Systems

Only a few object-oriented libraries manage sequential and parallel code reuse. In the context of large-scale distributed computing some numerical methods require sequential and parallel code reuse concurrently. We present how the use of component based approach and strict separation between control flow and data management can solve this problem. We propose a solution based on the integration of the LAKe library in YML scientific workflow. Our experiments on French GRID5000 platform valid the approach.

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CP20

Bounding the Dilation and Congestion of a Graph

For any *constraint* graph Z, a *Z-layout* of an input graph G is a mapping μ that maps vertices of G to distinct vertices of Z and also maps each edge uv of G to a $\mu(u)\mu(v)$-path of Z. The *Z-dilation* of G is

$$d_Z(G) = \min_{\mu} \max_{e \in E(G)} \mathit{length}(\mu(e)),$$

and the *Z-congestion* of G is

$$c_Z(G) = \min_{\mu} \max_{\alpha \in E(Z)} |\{e \in E(G) : \mu(e) \textit{ contains } \alpha\}|.$$

In particular, if Z is the two-way infinite path, then the Z-congestion and Z-dilation are known as *cutwidth* and *bandwidth*, respectively. In this talk, we present structural results on bounding these parameters when Z is the two-way infinite path, the complete infinite binary tree, the infinite planar grid, and, in general, the infinite d-dimensional grid. These structural results lead to efficient heuristics for computing these parameters.

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CP20
Power-Aware Frequency Balancing for Linear Algebra on Heterogeneous Grids

The power consumption in large scale high performance computational science is becoming a crucial consideration. Power efficiency optimization is an important goal for future supercomputer and grid programming. We propose a power-aware Lanczos-based eigensolver by means of Dynamic Voltage Scaling. We locally (resp. globally) saved up to 20% (resp. 9%) of energy on a power-aware cluster using the *PowerNow!* technology. We will introduce and discuss our recent work on frequency balancing and task scheduling strategies in order to save energy for some linear algebra methods on heterogeneous Grid or Cluster of clusters.

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CP20
Manufacturing Cell Formation Based on Graph Coloring

A method for cellular manufacturing formation is presented. The algorithm computes the dissimilarities between parts and organizes the production system in manufacturing cells. A graph is generated and a coloring algorithm is activated in order to obtain the desired number of cells. The results obtained on several examples found in the literature are consistently equivalent to or even better than those hitherto proposed, in terms of inter-cell moves and dimensions of the cells.

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CP21
Old and New Straight Line Detectors: Description and Comparison

We present several methods, old and new, used for Straight-line detection in an image. We begin by reviewing the Standard Hough Transform (SHT), then three new methods are suggested: the Revisited Hough Transform (RHT), the Parallel Axis Transform (PAT) and the Circle Transform (CT). These transforms utilize a point-line duality to detect straight lines in an image. To compare the methods we analyze the distribution of the frequencies in the accumulators and observe the effect on the detection of false local maxima. We also compare the robustness to noise of the four transforms. Finally an example with a real image is given.

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CP21
Generalized Radon Transforms in Electron Microscope Tomography

We report here on recent extensions to the electron microscope tomography code, TxBR, primarily intended for large-field images. These extensions include a general model for various data acquisition modes, a general bundle adjustment with improved alignment techniques, more accurate filters which compensate for curvilinear electron trajectories, and a fast nonlinear backprojection. In addition we discuss the algorithms implemented in this code in the context of the theory of Fourier integral operators.

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CP21
Evaluating the Relative Importance of the Terms of the Navier-Stokes Equations Utilizing Data from HF Radars

The relative importance of the terms of the Navier-Stokes equations was evaluated using information from HF radars for the Pacific U.S.-Mexico region. The set of equations obtained, describing the vertically averaged horizontal velocities, was evaluated using a time series of superficial velocities measured by HF radars in 2003. A computational algorithm calculated the relative contribution of each term and classified the area of the zones by means of dominate physical budgets.

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CP21

The Determination of the Support and Surface Conductivity of a Partially Coated Buried Object

An inverse problem for a partially coated anisotropic medium is considered. We construct the image of the target by a knowledge of Cauchy data on the boundary of a domain containing the obstacle. We then give a variational characterization of the supreme of the surface conductivity and validate the method with some numerical examples.

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CP21

Fast Solution of Nonlinear Bvps from Image Matching

We present, discuss and evaluate different numerical methods for the fast and robust solution of nonlinear elliptic bvps of second and fourth order. They arise as the Euler equations of variational principles in mono- or multimodal image matching. The corresponding regularized functional is nonconvex, has many local minima and up to 10^8 unknowns. We use Landweber, cg and Levenberg–Marquardt methods with fft and multigrid solvers combined with smoothing, multiresolution and trust region approaches.

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CP22

A Front-Fixing Finite Element Method for the Valuation of American Options

A front-fixing finite element method is developed for the valuation of American options on stocks. Stability and solution nonnegativity are established under some appropriate assumptions. Numerical results are presented to examine our method and to compare it with the other methods.

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CP22

Asymptotics of Barrier Option Pricing Under the CEV Process

We apply a singular perturbation analysis to options pricing under the constant elasticity of variance (CEV) assumption, which is also called the square root process. We consider also the CEV model with barriers, and this leads to a rich asymptotic structure. The analysis assumes that the variability is small, and employs the ray method of geometrical optics and matched asymptotic expansions.

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CP22

Hierarchical Approximation of Interest Rate Products Under Multi-Factor HJM Term-Structures of Interest Rates

We consider the valuation of interest rate products with effected cash flow under a multifactor Heath-Jarrow-Morton (HJM) model of the term-structure of interest rates by hierarchical approximation. At the higher-level, we apply a stochastic spectral approximation of the forward rates and exhaust an indexed family of regularized Hamilton-Jacobi characterizations of the value function. At the lower-level, we utilize penalization and an extrapolation method-of-lines finite element method. Application to interest rate caps and an American discount bond option are considered in order to demonstrate the applicability of the method.

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CP22

Numerical Valuation of American Options as Free Boundary Problems

Under the Black-Scholes model the price function of an American put/call option satisfies a time-dependent free boundary problem. Due to the smoothness properties Dirichlet and Neumann boundary conditions hold at the optimal exercise boundary which is the free boundary. After an implicit finite difference discretization the location of the boundary at each time step is found iteratively by solving PDEs in varying domains. This formulation leads to a more accurate approximation for the optimal exercise boundary than a more traditional linear complementarity formulation.

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MS0

Promoting, Publicizing and Publishing Undergraduate Research

Undergraduate research often produces exciting results that you want to share both on campus and with the larger mathematical community. We discuss effective strategies for promoting, publicizing and publishing undergraduate research. Local strategies include undergraduate research seminars and student webpages. We highlight national conference venues targeting student talks and posters. Fi-

nally, we introduce the electronic journal SIAM Undergraduate Research Online (SIURO) which is dedicated to promoting undergraduate research with rapid turnaround and a high profile.

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MS0

External Periodic Driving of Large Systems of Globally Coupled Phase Oscillators

Large systems of coupled oscillators subjected to a periodic external drive occur in many situations in physics and biology. Here the simple, paradigmatic case of equal-strength, all-to-all sine- coupling of phase oscillators subject to a sinusoidal external drive is considered. The stationary states and their stability are determined. Using the stability information and numerical experiments, parameter space phase diagrams showing when different types of system behavior apply are constructed, and the bifurcations marking transitions between different types of behavior are delineated. The analysis is supported by results of direct numerical simulation of an ensemble of oscillators.

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MS0

The Primitive Equations with Multiplicative Noise

The Primitive Equations are a fundamental model describing large scale oceanic and atmospheric processes. They are derived from the fully compressible Navier-Stokes equations on a combined basis of scale analysis and meteorological data. While an extensive body of mathematical literature exists in the study of these systems, very little is known in the stochastic setting. In this talk we discuss recent joint work with M. Ziane concerning existence and uniqueness of solutions in the presence of multiplicative noise terms.

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MS0

The Structure of Social Networks and Modeling the Spread of Infectious Disease

The modeling of the spread of infectious disease in humans relies both on the properties of the disease in question and the interpersonal contact within the host population. This study focuses on the importance of the structure of the social network in which a disease spreads. Older models assume that the population is homogenous, and thus results depend only on the relative virulence of the disease. A novel model is used, which incorporates a social network. The results show that the behavior of diseases is as much dependent on the social structure of the population. Various social network types were used in simulating infectious disease outbreaks, and the results confirm that social networks with different properties exhibit different behavior for the same disease. Because the research is based on a new model for the spread of disease, the properties of the model itself were fully explored as well.

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MS0

A Method For Catadioptric Imaging Sensor Design

We propose a method to design a catadioptric imaging sensor that will satisfy a given world-to-sensor mapping via solving a system of PDEs. We first solve for the projection , which the imaging sensor would realize. Then with this projection, we set up a set of differential equations for the mirror surface, which is the dioptric component of the catadioptric sensor. We present two examples of this construction.

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MS0

Mathematical Modeling of Electrostatic Interactions with Mean Curvature Surfaces

We investigate the interaction of static electric fields with surfaces of zero and constant mean curvature. These surfaces are of relevance in areas such as MEMS/NEMS, self-assembly, nanolithography, and microfluidic processes. Two particular systems are described. One involves a catenoid membrane deflected by an axially symmetric electric field. The other involves dynamics of collapsing bubble systems in the presence of electric forces. In each case the effect and utility of the electric field is examined.

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MS0

Structural Adaptation of Blood Vessels: Modeling,

Simulation, and Analysis

Structural adaptation of blood vessels is a physiological process through which the width and diameter of blood vessels change due to stimuli. We implement a model for structural adaptation proposed by Pries and Secomb that consists of a set of coupled di?erential equations for wall width and diameter. Using analytical and computational tools, we conjecture that there may exist one or more equilibria vessel structures for ?xed ?ow and ?xed pressure conditions. Additionally, we use concepts from dynamical systems to determine the stability of these equilibria and explore the parameter space that produces biologically realistic vessel structures.

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MS0
Environmental Evolutionary Graph Theory

I consider a simple spatial model of competition between two species. The environment is represented by a graph with red and blue vertices, which offer different levels of reproductive fitness to the two species. In general, the process appears to be difficult to analyze. However, in the case where the coloring of the vertices is a "proper' two-coloring, I show that these graphs are fair: neither species has an overall advantage.

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MS0
Effects of Localized Forcing on Driven Thin Liquid Films

Thin liquid films driven up an inclined plane by temperature- induced surface tension gradients have been the focus of extensive mathematical and experimental research. Using the lubrication approximation, the motion of a thin liquid film is described by a single fourth-order partial differential equation (PDE) that models the evolution of the height of the film. Such films are now known to exhibit both classical and non-classical wave structures. Bertozzi, Munch and Shearer first proved the existence of non-classical undercompressive waves in such films, and experimental evidence was provided by Cazabat, and later by Sur and Behringer. Levy and Shearer classified the types of wave structures emerging from a Marangoni- driven film. In a recent analytical and numerical study, Haskett, Witelski and Sur used localized Marangoni forcing to produce a "microfluidic valve" that provides control of a thin flow of Marangoni and gravity-driven viscous fluid. This work explores the development of classical and non-classical wave structures in the film, which appear as homoclinic and heteroclinic orbits in numerical simulations.

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MS0
Preconditioning the Lippmann-Schwinger Equations For Scattering By Thin Structures

We consider the efficient modeling of waves scattered by thin, inhomogenous obstacles. Such problems arise in the study of photonic band gap structures. We exploit asymptotic results related to the thinness of the obstacle to construct a preconditioner for the three dimensional problem that requires solving a system with complexity equal to a two dimensional problem at each preconditioning step.

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MS0
A Posteriori Error Estimates for Finite Volume Approximation of Elliptic Equations on General Surfaces

In this talk, we will present a residual-type a posteriori error estimator for finite volume discretization of steady convection-diffusion equations defined on general surfaces in R^3, where the surfaces may be implicitly represented as level sets of smooth functions. Reliability and efficiency of the a posteriori error estimator are rigorously proved. Some numerical experiments will also be tested to demonstrate our theoretical results.

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MS0
Panel Discussion on Running an Undergraduate Research Program

Speakers discuss their experiences and thoughts surrounding undergraduate research in dynamical systems, and answer audience questions.

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MS1

Methods for Optimal and Suboptimal Estmation

I will give an overview of recent work on optimal and suboptimal state estimation. In particular, I will discuss the problem of data assimilation for nonlinear stochastic dynamic equations. A variational method, a closure scheme, a mean-field approximation, and a path integral Monte Carlo approach will be discussed. Results for several sample problems will be given.

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MS1

New Horizons for the Estimation and Forecasting of Chaotic Systems

During the last 50 years, estimation techniques for nonlinear chaotic system have developed in parallel, and to some extent independently, in the controls and weather forecasting communities, with the former focusing on algorithm development, albeit mostly for small-scale systems, and the latter focusing on practical implementations in large-scale systems. A host of new, important applications may be analyzed with related tools, such as the forecasting of changes in ocean currents and temperatures, which in turn drive climate change, and the forecasting of contaminant release plumes in urban environments, for the coordination of emergence response to explosions (either intentional or accidental). These applications are facilitated by massive computational resources and advanced numerical algorithms becoming more and more readily available. This talk will survey some of these new opportunities for large-scale estimation and forecasting algorithms, some of the significant technical issues involved in addressing them effectively, and the potential for signifiant societal impact which these opportunities present.

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MS1

Particle Kalman Filtering and Data Assimilation in Meteorology and Oceanography

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

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MS1

The Local Ensemble Kalman Filter for Data Assimilation

Data assimilation refers to the problem of estimating initial conditions and parameters of a spatiotemporal dynamical system from noisy empirical measurements. The Local Ensemble Transform Kalman Filter (LETKF) is a state-of-the-art, model-independent framework for this estimation problem. I will survey recent applications to weather forecasting, including the operational U.S. Weather Service global forecast model as well as to oceanography, using the Estuarine and Coastal Ocean Model developed at Princeton University. The accuracy and computational efficiency of the LETKF also will be assessed.

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MS2

Fluid Avalanches on a Laboratory Scale

We will summarize theoretical approaches used to describe the motion of an avalanching mass down a steep slope. Focus is given to Newtonian and viscoplastic fluids. The governing equation can be obtained by assuming that the flow-depth to length ratio is small, which allows to simplifying a great deal the Navier-Stokes equations. Self-similar solutions to the governing equation can be worked out for early and late times. We compare our experimental data with these solutions.

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MS2

Coupling Between Driving Forces and Stress Gradients During Collapse of a Granular Column of Sand

Repeated measurements of the collapse of a column of granular sand are used to test mathematical models for granular flow, and provide a useful analogy to the physics of dry avalanches such as rock avalanches. In these experiments, variations in vertical acceleration of the column change the body forces driving the flow as well as the stresses resisting spreading of the granular material. Robust methods to estimated the changes in gravity wave speeds resulting from changes in vertical accelerations are crucial to capturing the behavior of the granular flow. An application of these methods to the active Ferguson rockslide currently endangering Merced Canyon in California will be presented.

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MS2

Generalizing Numerical Methods for Shallow Water Equations to Debris Flow Modeling

I will begin by presenting some numerical methods that we have developed over the last several years for modeling the shallow water equations, particularly in the context of tsunami modeling. These finite volume methods have some unique features for this application, such as well-balanced depth-positive-semidefinite Riemann solvers for inundation modeling, and adaptive mesh refinement. The focus of my talk will be on the benefits and difficulties of extending these methods to debris flows using the more general shallow-flow models developed by Iverson and Denlinger, which include stress terms from Coulomb friction and non-hydrostatic pressure.

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MS3

Refactoring Finite Element Computation

We examine several problems from finite element computation for which better mathematical abstraction has produced concrete improvement in both performance and code complexity.

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MS3

NSF Cyber Enabled Discovery (CDI) : Challenges for the Scientific Community

NSF CDI Objectives include the broadening of our Nation's capability for innovation by developing a new generation of computationally based discovery concepts and tools to deal with complex, data-rich, and interacting systems. With CDI, we expect to have enhanced ability to deal with research requiring petascale cyberinfrastructure, a strengthened technical basis for a new generation of computational discovery in all Science and Engineering, and significant progress in educating computational discoveries. This BOF hopes to address challenges facing languages, compilers, and operating systems in support of this venture. Examples include addressing Proebsting's Law and software keeping up with Moore's Law, verification of scientific software both semantically and operationally, co-design of machines in support of scientific software, symbolic, numeric, and algebraic software systems, team building, education and research training, as well as issues of how to address changes required in academia is support of these goals.

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MS3

Energy-Aware Sparse Scientific Computing

We consider sparse scientific computing applications on advanced architectures including multicore multiprocessors. We first discuss iso-efficient scaling with respect to the performance of the application and the energy consumed by the hardware. We then continue with strategies that can be applied at the interface of the application and the hardware to enhance performance and energy efficiencies.

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MS3

Performance Modeling: Understanding the Past and Predicting the Future in HPC

In the context of High Performance Computing, a performance model is a calculable expression that takes as parameters attributes of application software, input data, and target machine hardware (and possibly other factors) and computes, as output, expected performance. Via parameterization, performance models enable exploration of performance as a function of possible enhancements to machine or code, and can thereby reveal greater understanding of the performance, as well as the opportunities to improve it.

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MS4

Tapenade: Automatic Differentiation of Fortran and C

We present Tapenade, a tool for Automatic Differentiation (AD) of programs by source transformation. We illustrate tangent and reverse modes of differentiation on short examples. We show how specific static data flow analysis is used to improve the differentiated source. Until recently, Tapenade could differentiate only Fortran95 programs. We present the implementation choices of Tapenade, and how they made it easier to accept C programs as well. We conclude presenting some large scale applications.

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MS4

OpenAD: Automatic Differentiation for Fortran

Not available at time of publication.

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MS4

Recent Developments of AD for MATLAB

We give an overview of AD-tools for MATLAB, concentrating on the source transformation tool ADiMat. In particular, we report on recent advances in code optimization for dynamically implictly typed languages.

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MS4

ADOL-C: Automatic Differentiation of C/C++ code

After a short introduction to Automatic Differentiation (AD), We present the AD-tool ADOL-C for the differentiation of C and C++ codes including a short description of its application. Adol-C can handle codes based on classes, templates and other advenced C++-features. Recent developments, including the treatment of iterative processes and functions evaluated in parallel, are discussed. Finally, some examples covering aerodynamics and the computation of quantum-plasma illustrate the potential of ADOL-C.

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MS5

Brownian Ratchets Driven by Asymmetric Hydrolysis

We develop a simple one-dimensional model for track-induced molecular motion. In contrast to molecular motors that invoke a molecular conformational change to power their biased motion, examples of track-propelled motion arise in biophysical settings such as enzymatic processing of collagen and motion of DNA junctions. Our simple model describes track-propelled motion in terms of asymmetric nucleation of hydrolysis waves by coupling motion of a load particle to moving domain walls. We use asymptotic analysis in a moving frame to compute the dependence of the motor velocity as a function of local hydrolysis rates and find a maximum velocity at intermediate nucleation asymmetries.

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MS5

Molecular Motors Interacting with Their Own Tracks

Dynamics of molecular motors that move along linear lattices and interact with them via reversible destruction of specific lattice bonds is investigated theoretically by analyzing exactly solvable discrete-state "burnt-bridge" models. Molecular motors are viewed as diffusing particles that can asymmetrically break or rebuild periodically distributed weak links when passing over them. Our explicit calculations of dynamic properties show that coupling the transport of unbiased or biased molecular motors with the bridge-burning mechanism leads to a complex dynamic behavior. It includes dynamic transitions, strong and suppressed fluctuations and the reversal of the motion direction. Dynamics of the system is discussed in terms of the effective driving forces and transitions between different diffusion regimes.

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MS5

Einstein Relation and Effective Diffusion of Molecular Motors

In recent years, single molecule experiments provided measurements on the stochastic time series of motor position under various external conditions. This allows us to examine not only the average velocity but also the effective diffusion of a motor as a function of external conditions. However, to correctly interpret and utilize the data on effective diffusion, we need to first understand theoretically the behavior of effective diffusion. In this presentation, we study the effective diffusion of a Brownian particle in a static periodic potential.

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MS5

The Shape and Dynamics of the Spirochetes

In this talk I will discuss the shape and motility of a unique group of bacteria, the spirochetes. These bacteria use helical polymer filaments (flagella) encased between their cell wall and outer membrane to maintain their cell shape and to drive motility. Consideration of the coupling between the cellular and flagellar elasticity leads to a model that describes the shape and dynamics of a number of these bacteria, such as *Borrelia burgdorferi* and the *Leptospiraceae.*

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MS6

Multiscale Simulation of Copper Electrodeposition

Copper electrodeposition is widely used to fill on-chip interconnects and vias in the fabrication of computer processors. Simulation of the electrodeposition process is challenging due to the structure of the electrolyte mass transport model, the need for resolution at the smallest scales, and the difficulty of coupling electrolyte and surface simulations. We describe a new numerical algorithm that is much more efficient than previously developed methods, scales well with grid refinement and is naturally parallelizable.

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MS6

Multiscale Methods for Coulomb Collisions in Plasmas

This presentation describes a hybrid computational method for Coulomb collisions in a plasma that combines a Monte Carlo particle simulation and a fluid dynamic solver in a single uniform method throughout phase space. The new method is based on a hybrid representation of the velocity distribution function $f(v)$, as a combination of a Maxwellian equilibrium $M(v)$ and a collection of discrete particles $g(v)$. The Maxwellian M evolves in space and time through fluid-like equations, and the particles in g convect and collide through Nanbu's Monte Carlo particle method (PRE 1997). Interactions between M and g are represented by a thermalization process that removes particles from g and includes them in M and a dethermalization process that samples particles from M and inserts them into g. As test cases for the hybrid method, we have used evolution of a bump-on-tail.

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MS6

Operator Decomposition Solution of Nonlinear Coupled Elliptic Systems

We present an a posteriori error analysis and adaptive framework for the operator decomposition solution of nonlinear coupled elliptic systems. This solution technique requires iteration, and we provide estimates for both the iteration error and the main components of the non-iteration error. The adjoint method used for error control also may be solved using operator decomposition. We discuss implementation issues and give several examples demonstrating the different features of the error control framework.

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MS6

Convergence of Multiscale Numerical Methods for Flow Problems

Multiscale numerical methods are used to solve flow problems when the permeability, i.e., coefficient in the elliptic operator, is heterogeneous. We show that a popular multiscale finite element method fails to reproduce constant flow fields in certain cases, and numerical examples for which the method fails to converge in any meaningful way. The problem arises when the microstructure leads to a tensorial homogenized permeability. A modified method is shown to converge with respect to the microstructure.

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MS7

Learning in a Biophysical Network: Constraints Set by Population Oscillations

Experiments in insect antennal lobe (AL) show that population activity exhibits a strong oscillatory component, whereas individual cells are not oscillators. We propose to use as a model of the AL an idealized excitatory-inhibitory network, generating population oscillations from non-oscillatory noisy elements. Tuning the network into the right frequency regime suggests constraints on the network connectivity. Qualitatively matching the observed learning-induced changes in oscillation properties, suggests how the network parameters are affected by learning.

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MS7

Propagation of Information in Correlated Feedforward Networks

Spike train correlation enhances the propagation of activity in spiking neural networks, but limits the coding capacity of a network through redundant processing. We show that when the correlation and firing rate of a presynaptic network co-vary with one another, the transfer of information (measured in the Fisher sense) to a postsynaptic population is significantly enhanced. These results show that even when spike correlations do not themselves code input stimuli, they can determine the efficacy of propagated rate-based codes in the nervous system.

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MS7

Multiplexing Information in Neural Codes on Multiple Timescales

Stochastic methods provide a means to connect dynamical descriptions of neuronal behavior with their coding properties, expressed in the language of systems neuroscience through receptive fields and thresholds. We show how neuronal biophysical properties determine the feature selectivity of neurons with respect to rapid temporal input fluctuations. Further, at longer timescales neurons encode slowly varying statistical properties of the fluctuating input. The form of this encoding is also determined through biophysical properties.

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MS7

Democratization and Information Processing in Dendrites

One way to achieve amplification of distal synaptic inputs on a dendritic tree is to scale the amplitude and/or duration of the synaptic conductance with its distance from the soma. This is an example of what is often referred to as "dendritic democracy". Although well studied experimentally, this phenomenon has not received much attention from mathematicians. A passive model of a dendritic tree with distributed excitatory synaptic conductances will be presented and a number of key measures of democracy analyzed. In the second part of the talk I will discuss the clusteron, a model neuron that learns by spatial rearrangements of its synaptic inputs.

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MS8

Non-Iterative Methods in Discrete and Continuous Random Settings

We develop sufficient conditions for applicability of Dijkstra-like algorithms to an important subclass of finite-state deterministic infinite-horizon problems. We use these results to build efficient (non-iterative) numerical methods for a related class of static Hamilton-Jacobi partial differential equations. Our approach is illustrated using optimal idle-time control problems on discrete and continuous state spaces.

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MS8

Maximizing the Reliability of On-Time Arrival in a Stochastic Network

This presentation focuses on the problem of finding an optimal routing strategy to maximize the probability of arriving at the destination within a time threshold. Dynamic programming based formulation is proposed for such a problem, which has advantages of accommodating real-time information and improving numerical efficiency. This work is applicable to fields involving stochastic networks such as transportation and computer networks.

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MS8

Relatives of Static Hamilton-Jacobi: Algorithms and Updates

We describe several algorithms based on dynamic programming (DP) for problems of the minimum cost to go variety. First, we show how to marry a viability kernel with a label setting algorithm to more efficiently approximate discontinuous minimum cost to go solutions. Second, we show how a two stage DP algorithm can efficiently solve multi-location rendezvous scenarios. Third, we describe an algorithm with improved dimensional scaling for a restricted class of dynamics.

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MS8

New Applications of Fast Eikonal Solvers

In recent years, Dijkstra-like solvers, borrowed from discrete network flow problems, have been extended to a large collection of continuous PDE problems. Our goal is to discuss a variety of new applications of the fast Eikonal and ordered upwind solvers. We shall discuss applications to medical segmentation, terrain mapping, image analysis, and wave propagation, including some new algorithms for computing higher dimensional problems.

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MS9

Parameterization for Mesoscale Ocean Transport through Random Flow Models

We describe a mathematical approach based on homogenization theory toward representing the effects of mesoscale coherent structures, waves, and turbulence on large-scale transport in the ocean. We are developing a systematic parameterization strategy by building up deterministic and random subgrid-scale flow models in an increasing hierarchy of complexity, coupling the results from numerical simulations of cell problems with asymptotic analysis with respect to key nondimensional physical parameters.

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MS9

Multi-scale Ocean Modeling with Adaptive Mesh Methods

A particular challenge in the numerical simulation of ocean dynamics is the vaste range of length scales that play a role. In this presentation a modelling approach based on adaptive mesh and finite element techniques will be presented that is new in ocean modelling. Some of the challenges in applying these techniques to geophysical problems will be highlighted. Work on model validation will be shown as well as application of this in real world problems.

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MS9

Particles in a Stochastic Flow with a Linear Drift

We consider a stochastic flow with a deterministic drift linearly depending on the space coordinate (linear shear flow). Conditions are found for existence of the inertial regime in such a flow. The diffusivity tensor is computed in terms of the shear and fluctuation statistics. Next, the relative dispersion is discussed for both local and non-local dynamics in the framework of the suggested model.

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MS9

Wave-Breaking Dissipation in Wave/Current Interactions

We propose a stochastic parametrization for dissipative mechanisms at wave scales. This parametrization is then used to integrate wave breaking and white capping into a wave-current interaction model. This presents a significant improvement in the ability of the model to represent realistic oceanic flows, and further, answers the question of how and why breaking will lead to dissipation at the longer spatio-temporal scales of currents. There are two advantages to this approach: it makes better contact with field data, when compared to complex closure/turbulence models, and it has a theoretical analogy to the process of representing diffusion in other systems via Langevin-like equations.

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MS10

Network Security in Models of Complex Networks

The game of Cops and Robber is a widely studied discrete-time game played on graphs, which supplies a model for security in real-world complex networks such as the web graph. An unexplored direction of research is to analyze the cop number in stochastic models of complex networks. As a first step in this direction, we provide asymptotic bounds for the cop number of the random power law graphs introduced by Chung and Lu.

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MS10

Structure and Evolution of Online Social Networks

Online social networks have become major and driving phenomena on the web. In this talk we focus on the properties of two large online social networks, namely, the LiveJournal network of friends and the Flickr network of contacts. In the context of LiveJournal, we formulate a simple and general model of social networks that can explain the success of Milgram's famous experiment that gave rise to 'six-degrees of separation'. In the context of Flickr, we focus on the temporal evolution of social networks from a graph-structure point of view.

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MS10

Diameters of Random Spanning Trees for Complex Graphs

Kleinberg observed the diameter of random sub-trees in some social networks G is much larger than the diameter of G itself. Motivated by his observation, we studied the diameter of random spanning trees in a complex graph G. Under some weak conditions, we give bounds on the diameter of random spanning trees in term of a few graph parameters, namely the average degree d, the second order average degree $\tilde{d}$, and the mixing rate σ of random walks on G. Our results is consistent with Kleinberg's observation.

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MS10

Generative Models for Scalefree Networks Using Different Ranking Schemes

The occurrence of power law degree distributions in self-organizing networks such as the web graph is often explained by a model based on the principle of Preferential Attachment. In such models, vertices are linked to by a newly added node with probability proportional to their degree. We show that a more subtle control of the power law behaviour can be obtained if the preferential attachment is based on a ranking of the vertices according to their degree. This rank-based approach was first proposed by Fortunato, Flammini and Menczer. We have extended the rank-based attachment scheme to a variety of ranking schemes: vertices can be ranked by degree, according to a prestige label, or each new vertex can be assigned a random rank. It turns out that many of these schemes produce a power law degree distribution, with an exponent that can be controlled by the strength of the attachment. This makes rank-based attachment an plausible mechanism behind the occurrence of power laws in many real-life networks.

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MS11

A General Perfectly Matched Layer Model for Hyperbolic Parabolic Systems

In this seminar will we will present how our (Hagstrom, Kreiss and A) general model for hyperbolic systems can be extended to hyperbolic-parabolic systems. The importance of the perfect matching property will be clearly illustrated by numerical experiments performed for two linear applications: an advection-diffusion equation and the linearized Navier-Stokes equations. We end by presenting the non-linear version of our PML and its application to the compressible Navier-Stokes equations.

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MS11

Fast Non-local Non-reflecting Boundary Conditions for Wave Scattering Problems

We present and demonstrate a new methodology for evaluation of computational boundary conditions in three-dimensional space. The proposed algorithm, which is accurate, numerically convergent and fully nonlocal, is based on two novel concepts: Equivalent-Source Representations and Continuation Fourier Series. With a computational cost significantly smaller than that of an underlying volumetric solver, the algorithm allows for selection of computational boundaries lying arbitrarily close to the scatterer for scatterers of arbitrary shape.

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MS11

Grid Anisotropy and Stability of a Perfectly Matched Layer

Numerical experiments have shown that PML solutions on curvilinear grids (non-regular Cartesian meshes) exhibit long time numerical instabilities. In 2003, Becache et al. used dispersion relations (slowness curves) of continuous models to predict instabilities in PML solutions. In this work the same analysis was used on the semi-discrete problems to show that on certain anisotropic meshes numerical instability may be inevitable. Our numerical experiments confirmed that a PML that is stable on a regular Cartesian grid may exhibit long time instability on skewed meshes. The instability introduced by the anisotropy of the mesh is weak, and it could be eliminated by the addition of accurately constructed artificial dissipation.

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MS12

Strong Stability Preserving Time-Stepping Methods

SSP time discretizations were developed to ensure nonlinear stability properties in the numerical solution of hyperbolic PDEs with discontinuous solutions. SSP methods preserve the strong stability properties of the spatial discretization coupled with first order Euler time stepping. In this talk we describe the development of SSP methods, optimal explicit and implicit SSP Runge-Kutta and multistep methods, for linear and nonlinear problems. We also discuss the SSP properties of spectral deferred correction methods.

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MS12

Practical Considerations for IMEX SSP Runge-Kutta Methods

Over the last years, a great effort has been done to develop Runge-Kutta (RK) methods $(\mathcal{A}, b^t)$ preserving qualitative properties (e.g. contractivity, monotonicity or positivity) for the exact solution of ordinary differential systems. Some results available in the literature ensure these properties under certain stepsize restrictions given in terms of the radius of absolute monotonicity of the RK method $\mathcal{R}(\mathcal{A}, b^t)$. Nowadays there is a deep knowledge on $\mathcal{R}(\mathcal{A}, b^t)$ for explicit RK methods and a great interest in the construction of implicit RK schemes with large values of $\mathcal{R}(\mathcal{A}, b^t)$. However, these results are given for the exact numerical solution whereas in practice, for implicit schemes, the numerical solution available is only an approximation of it. A potential interest of these implicit SSP RK schemes is their use for the construction of SSP IMEX RK methods. In this context, order barriers and structure restrictions for IMEX schemes should be taken into consideration when implicit SSP RK methods are constructed. In this talk we will give some practical considerations for IMEX SSP Runge-Kutta methods focusing on effective stepsize restrictions for implicit SSP RK schemes, and order barriers and structure restrictions for IMEX RK methods.

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MS12

Generalizations of Positivity and Strong Stability Preservation

We reformulate positivity and SSP of Runge-Kutta and linear multistep methods in a unified setting, using forward invariance of convex sets of discrete dynamical systems. We derive explicit formulas for time-steps corresponding to the discrete forward invariance of arbitrary closed, convex sets. We show that for appropriately constructed convex subsets the time-step thresholds which guarantee their discrete forward invariance are much larger than that resulting from the classical theory. Finally, we illustrate our results by computational experiments.

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MS12

Optimal Explicit and Implicit SSP Runge-Kutta Methods

We consider the problem of finding explicit and implicit Runge-Kutta methods with optimal SSP timestep restrictions. Using an alternative formulation of the associated optimization problem, we find new methods by numerical search. The explicit methods have efficient low-storage implementations. The implicit schemes all have an efficient diagonally implicit structure. Our results include families of second and third-order methods that achieve the maximum theoretically achievable effective SSP coefficient, as well new, more efficient higher-order methods.

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MS13

General Solutions of the Stokes Equations and an Application to Singularity Driven Flows Inside an Arbitrary Body

We discuss some general solutions of steady Stokes equations. We discuss a new method developed to study a singularity driven Stokes flow inside an arbitrary body. Since this technique gives an analytic, although approximate method to find the solution, it is more useful compared to other previously known numerical techniques.

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MS13

Optimization of the Hydrodynamic Process of Fuel Feeding into a Diesel Cylinder

The process model is described by the differential equation of a viscous fuel flow in a pressure pipelining with boundary conditions, which are specified for the inflow and outflow faces. The optimization procedure and the stability evaluation of an optimal solution, which allows for model errors, are presented. The method of identification of the stability domain boundaries is described. The search algorithm of a least sensitive solution and an example of its application are presented.

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MS13

General Solutions of the Navier-Stokes Equations and the Vorticity Transport Equations in the Lamb Variables

General topological solutions of the Navier-Stokes equations and the vorticity transport equations are constructed in the Lamb variables by using the unsteady Boussinesq-Rayleigh-Taylor series in various dimensions. It is shown that are forced and free solutions the Navier-Stokes equations and there is only a free solution of the vorticity transport equations. The basic nonlinear eigen modes of the general topological solutions of the Navier-Stokes equations in the Euler and Lamb variables are compared.

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MS13

A New Method of Visualization of Unsteady Coherent Structures in Three Dimensions

A novel method of imaging of unsteady vector fields in three dimensions is considered, which continues the classical two-dimensional method of visualization of coherent structures by isocurves of the stream function. The method that is based on numerical integration of isochronous three-dimensional vector lines identifies and displays multiscale vector structures by open and closed moving surfaces, the transversal size of which is proportional to the magnitude of the vector field. Examples of visualization of multiscale vortex and wave pairs of a mixing model, which is computed by the general topological solution of the Poiseuille flow, are provided for various Reynolds numbers.

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MS13

Some New General Solutions of the Steady and Unsteady Oseen Equations

We discuss some solutions of steady Oseen equations that have been previously available. We present a new solution of Oseen equations that has been proposed recently by us and discuss the importance of this new solution. We also discuss a new general solution of unsteady Oseen equations both in the absence of body forces as well as in the presence of body forces.

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MS14

EnVE: A Consistent Hybrid Ensemble/variational Estimation Strategy for Multiscale Uncertain Systems

Chaotic systems are characterized by long-term unpredictability. Existing methods designed to estimate and forecast such systems, such as Extended Kalman filtering (a "sequential" or "incremental" matrix-based approach) and 4Dvar (a "variational" or "batch" vector-based approach), are essentially based on the assumption that Gaussian uncertainty in the initial state, state disturbances, and measurement noise leads to uncertainty of the state estimate at later times that is well described by a Gaussian model. This assumption is not valid in chaotic systems. A new method is thus proposed that combines - the speed and LQG optimality of a sequential-based method, - the non-Gaussian uncertainty propagation of an ensemble-based method, and - the favorable smoothing properties of a variational-based method. This new approach, which we refer to as Ensemble Variational Estimation (EnVE), is a direct extension of algorithms currently being used by the weather forecasting community. EnVE is a hybrid method leveraging - sequential preconditioning of the batch optimization steps, - simultaneous backwards-in-time (a.k.a. "retrograde") marches of the system and its adjoint (eliminating the storage difficulty and/or checkpointing normally associated with 4Dvar), - a receding-horizon optimization framework, - adaptation of the optimization horizon based on the estimate uncertainty at each iteration, and - repopulation of the ensemble based on the sensitivities determined during the adjoint analyses. If the system is linear, EnVE is consistent with the well-known Kalman filter, with all of its well-established optimality properties. The strength of EnVE is its remarkable effectiveness in highly uncertain nonlinear systems, in which EnVE consistently uses and REVISITS the information contained in recent observations with batch (that is, variational) optimization steps, while consistently propagating the uncertainty of the resulting estimate forward in time.

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MS14

Large-Scale Data Assimilation in Hydrogeology via Statistical Parametrization

By using homogeneization techniques we can characterize the uncertainty in hydrological flows in heterogeneous media. This enables us to propose a large-scale hydrogeomorphological model that takes into account the smaller scales in a statistically-rigorous manner. The model is then used in a Bayesian framework to incorporate measurements of the substrate as well as the hydraulic head, including its inherent measurement errors, to produce an estimation technique that yields the large scale flow, an estimate of the mean and uncertainty of the boundaries between materials with different conductivities and the conductivities themselves. By careful choices we have been able to retain the classical form of the flow equations which then allow us to use widely available optimized elliptic solvers. We also use convex likelihood functions that allow us to use existing efficient Newton-based optimization methods.

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MS14

Second Order Adjoints in Atmospheric Inverse Modeling

Atmospheric chemical transport models (CTMs) are essential tools for the study of air pollution, for environmental policy decisions, for the interpretation of observational data, and for producing air quality forecasts. Many air quality studies require sensitivity analyses, i.e., the computation of derivatives of the model output with respect to model parameters. While the traditional (first order) adjoint models give the gradient of the cost functional with respect to parameters, second order adjoint models give second derivative information in the form of products between the Hessian of the cost functional and a user defined vector. We discuss the mathematical foundations of the discrete second order adjoint sensitivity method and present a complete set of computational tools for performing second order sensitivity studies in three-dimensional atmospheric CTMs. Numerical examples illustrate the use of these computational tools in important applications like sensitivity analysis, optimization, uncertainty quantification, and the calculation of the directions of maximal error growth.

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MS14

Flow-dependence of the Performance of an Ensemble-based Analysis-forecast System

Data assimilation is problem at the intersection of dynamical systems theory and mathematical statistics. In this talk, we focus on the dynamical systems aspects of the problem. In particular, we argue that most techniques of dynamical systems theory, which have already been applied to geophysical fluid dynamical systems, have a solid theoretical foundation only for low-dimensional systems. Since geophysical fluid dynamical systems are inherently high-dimensional, a systematic approach to extend the theoretical machinery to increasingly more complex systems would be highly desirable. In this talk, we outline one potential approach to address this issue: the high-dimensional system is viewed as the collection of local systems; the local state vector is defined by the variables of the original high-dimensional system from a local neighborhood of each physical location; and properties that smoothly vary with the location are computed based on the local state vectors. This approach motivated our research group to develop the Local Ensemble Transform Kalman Filter (LETKF) data assimilation scheme and it can also be used to explain the spatio-temporal variability of the performance of an ensemble-based analysis-forecast system.

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MS15

Modeling Rain-induced Landslide Initiation from Wetting of Dry Soil to Failure using a Multiphase MPM

Modeling landslides requires consideration of solid and fluid phases throughout the process. Both phases undergo mixing (wetting), combined dynamic action, and separation (sedimentation and drying). Typically, each state is characterized by specialized differential equations, thus introducing difficulties in modeling transitions between states. The proposed approach attempts to unify all states and capture transition effects by modeling fluid and solid as distinct phases and producing physically meaningful behavior through respective interaction forces and discrete balance laws.

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MS15

High Mobility of Erosive Granular Flows and Surge Generation

The origin of the high mobility of natural granular flows is a challenging question for risk assessment. We investigate here the effect of erosion on avalanche mobility using the new partial fluidization model [Aranson and Tsimring, 2002]. We show that the presence of a very thin layer of granular material lying on the topography strongly increases flow mobility. As the thickness of the layer increases, travelling wave (i. e. surges) are generated as observed experimentally.

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MS15

Simulating Viscoplastic Avalanches

We present a comparison between experiment and numerical results for the dam-break problem involving viscoplastic fluids. The laboratory experiment consists in releasing a fine volume of a viscoplastic fluid down inclined plane and tracking the evolution of the free surface. A finite volume, two-phase *Navier-Stokes* solver was extended to treat fluids with shear-rate dependent viscosity. A semi-implicit *Chorin's projection scheme* in combination with a *bi-conjugate gradient* method is used.

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MS15

Modeling the Generation of Tsunami by Slides: Hydrocode Modeling

Understanding tsunami by landslides as the next challenge for hazard, risk and mitigation: Insight from multimaterial hydrocode modeling Sliding bodies, either traveling inside the water column or impacting into water, generate waves. Depending on the volume, velocity, and material properties of the moving mass, waves of significant height and length are generated. Such waves can be considered tsunami waves, even if their characteristic is profoundly different from classical tsunami generated by earthquakes. Most models of landslide-induced tsunami waves focus on the propagation of the generated waves as they are non-linear and require the application of higher-order terms in the governing equations. The actual generation process in these models is often simplified and tuned to two specific scenarios that can be realized in laboratory experiments: (1) the sliding body is represented by a rigid or (2) a viscous body. In real landslides, the rheology of the sliding body is unknown and varies between these two end-member scenarios. We present new modeling results to gain a better understanding of the relevant parameters affecting the characteristic of generated tsunami waves by landslides. The applicability of the multi-material hydrocode iSALE we used in our models is demonstrated by reproducing experiments conducted with rigid and viscous sliding bodies. Our results provide new insight of the slide dynamics, the coupling between the sliding body and the slope and the water column, repsectively. They confirm the known positive effect of increased velocity and increased volume of the sliding body on the initial wave characteristics. In addtion we have investigated how the rheological properties of the sliding body affect the wave characteristic.

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MS16
Advice for PhD Students and Postdocs Looking for Jobs

The first half of talk is loosely based on a recent news article on CNN titled '5 big mistakes new grads make'. Their advice given is good and some modifications can translate into advice for graduating PhDs and postdocs. The second half of the talk is more specific to the mathematical profession. Topics for discussion include: (a) the role of the thesis advisor and postdoc mentor in assisting with the job search; (b) what to put and not to put on your web page; (c) networking; (d) common courtesies such as when to say "thank you"; (e) voicemail greetings; (f) use of mathjobs.org; (g) applying for fellowships; (h) letters of recommendation and application review; (i) when to take a second postdoc; (j) deadlines and contingencies.

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MS16
Working as a Mathematician in Industry

An industry career in Mathematics can be both fun and rewarding. I will discuss the important components of a successful mathematics career: how to communicate ideas to non-mathematicians from upper management to those with limited educational background, methods for "hiding" the math, how to find projects of interest, prioritizing and managing time, working on crossfunctional teams, benefits and pitfalls of working with academia, marketing work internally, and most importantly, how to learn from your mistakes.

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MS16
No!!!!!

No is a powerful word that can change your life. When should you use it and when not? How can you say it most effectively? This talk will discuss some of the speaker's hard-earned lessons and her continuing education in this area.

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MS17
Single-Molecule Force Spectroscopy: Theory, Analysis and Interpretation.

Mechanical forces are generated during nearly every facet of the cell cycle. Recent advances in experimental techniques enable experimentalists to exert forces on individual molecules and observe their response in real time. The single-molecule approach has changed the way many physical, chemical and biological problems are addressed. We present an analytically tractable theory for extracting kinetic information from single-molecule pulling experiments at constant force or constant loading rate. Our procedure provides estimates of not only i) the intrinsic rate coefficient and ii) the location of the transition state, as in the widely used phenomenological approach based on Bells formula, but also iii) the free energy of activation. We illustrate the use of our approach by applying it to sets of data obtained from nanopore unzipping of individual DNA hairpins and from unfolding of single protein molecules with the atomic force microscope.

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MS17
Statistical Inference Techniques for Molecular Motors

While there has been significant strides in recent years in both modeling of and data collection methods for molecular motors, a gap remains in connecting these disciplines. This talk will include a survey of inference methods tying data to models. In addition, novel maximum likelihood methods for motor models will be introduced along with relevant data examples.

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MS17
A Step Toward Reconstructing Bond Potential Profiles

In many single molecule experiments on bond breaking, only a histogram of breaking time and/or breaking force can be observed. The process of bond breaking is classically modeled as the escape of a Brownian particle from a potential well. The profound mathematical question is whether or not it is possible and how to deduce information on the potential well from breaking time and/or breaking force distributions. In this talk, we explore this problem.

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MS17

Understanding an Intermediate Structure During Microtubule Assembly with Stochastic Simulations

Microtubules are one of the three kinds of cytoskeleton components. They are macromolecules with about 13 protofilaments formed with the $\alpha\beta$-tublin dimers. Microtubules play important roles in many eukaryotic cellular processes, including intracellular transporting, cell motility, meiosis and mitosis. According to the widely accepted textbook mechanism, during the assembly process the $\alpha\beta$-tublin dimers add onto the growing end of a microtubule one by one. However, Some experimental observations challenge this conventional view. This alternative model proposes that tublins first form a two-dimensional open sheet, which in turn closes into tubes. Cryo-EM studies show that within the two-dimensional sheet structure, two types of lateral interactions alternate between neighboring protofilaments. The experimental observations raise several questions. How can the sheet with alternating lateral interactions be formed? If the sheet structure is indeed the intermediate of microtubule assembly in vivo, is there any biological function for it? I will discuss our efforts of using stochastic modeling to address these questions.

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MS18

Volume Corrected Characteristic Methods

The characteristics-mixed method transports mass along the characteristic curves of the hyperbolic part of the equation, and thereby produces little numerical dispersion, conserves mass locally, and can use long time steps. Since the shape of a trace-back region is approximate, its volume may be incorrect, giving inaccurate concentration densities. We present a simple modification that conserves both mass and volume of the transported fluid regions. Theoretical convergence results and several numerical examples are given.

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MS18

Ordering-based Approaches for Improving Solver Efficiency in Reservoir Simulation

We propose a phase-based potential ordering of the equations and variables in fully implicit black-oil models. By exploiting flow direction information, this ordering gives rise to a more robust nonlinear solver that can circumvent the convergence difficulties experienced by Newton's method when large time steps are used. The ordering also benefits the linear solver by improving the convergence of the Constrained Pressure Residual (CPR) preconditioner and reduces its sensitivity to flow configurations.

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MS18

Robust Multi-D Upwind Methods that Reduce Grid Orientation Effects

We investigate truly multi-D upwind schemes for simulating adverse mobility ratio displacements. Modified equations analysis is used to predict the behavior of existing schemes, and we present a conservative, multi-D framework for designing positive upwind schemes for general velocity fields. We then develop a novel scheme with minimal constant transverse diffusion. Results for miscible gas injection demonstrate that multi-D schemes, and in particular our new scheme, reduce grid orientation effects as compared to dimensional upwinding.

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MS19

Multiscale Issues in the Simulation of Transport in Tokamaks

Radial transport of particles, heat, and momentum is a fundamental process limiting tokamak performance. The transport is generally the result of plasma microturbulence, which has a broad range of length and time scales, shorter than, but not always well-separated from, those of the transported (averaged) quantities. Various additional processes contribute, further broadening the range of scales. We survey the processes, and discuss the approaches used to bridge the scales. *Work performed for U.S. D.O.E. by LLNL under contract DE-AC52-07NA27344

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MS19

Modeling and Simulation of the Critical Nuclei Morphology in Solid State Phase Transformations

We present a diffuse interface model to study the morphology of critical nuclei during solid to solid phase transformations. It takes into account the anisotropic interfacial energy as well as the anisotropic long-range elastic interactions. It is demonstrated that the morphology of critical nuclei in cubically anisotropic solids can be efficiently predicted by the computational model without a priori assumptions. The effect of elastic energy contribution on the size and shape of a critical nucleus is studied. It is shown that strong elastic energy interactions may lead to critical nuclei with a wide variety of interfaces.

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MS19

Computational Environments for Modeling Carbon Sequestration

Geologic sequestration is proven to be a viable means of CO2 emission reduction and permanent storage. Modeling and prediction of the long-term movement as well as risk of escape of CO2 will require assimilation of huge datasets into simulators, incorporating coupled models that capture the physics of the system. We present a "wish list" for simulator capabilities as well as describe software developed at UT-Austin.

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MS20

Coupled Electric-Field Sensors

It is well known that overdamped unforced dynamical systems do not oscillate. However, well-designed coupling schemes together with the appropriate choice of initial conditions, can induce oscillations (corresponding to transitions between the stable steady states of each nonlinear element) when a control parameter exceeds a threshold value. In recent publications, we demonstrated this behavior in a specific prototype system, a soft-potential mean-field description of the dynamics in a hysteretic "single-domain' ferromagnetic sample. These oscillations are now finding utility in the detection of very weak "target' magnetic signals, via their effect on the oscillation characteristics, e.g. the frequency and asymmetry of the oscillation waveforms. In this paper we explore the underlying dynamics of a related system, coupled bistable "standard quartic' dynamic elements; the system shows similarities, but also significant differences from our earlier work. DC as well as time-periodic target signals are considered; the latter are shown to induce complex oscillatory behavior in different regimes of the parameter space. In turn, this behavior can be harnessed to quantify the target signal.

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MS20

Coupled-Core Fluxgate Magnetometers

Coupling-induced oscillations in a homogeneous network of overdamped bistable systems have been previously studied both theoretically and experimentally for a system of N (odd) elements, unidirectionally coupled in a ring topology. In this work, we extend the analysis of this system to include a network of nonhomogeneous elements with respect to the parameter that controls the topology of the potential function and the bistability of each element. In particular, we quantify the effects of the nonhomogeneity on the onset of oscillations and the response of the network to external (assumed to be constant and very small) perturbations, using our (recently developed) coupled core fluxgate magnetometer as a representative system. The potential applications of this work include signal detection and characterization for a large class of sensor systems.

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MS20

Coupled SQUID Sensor Systems

Recently, there has be a growing interest in coupled SQUID devices in the science community. The focus of this work covers theoretical and numerical computations which exploits well-designed coupling schemes to modeling the dynamics of the device. As a prototype, we study an array of dc superconducting quantum interference device (SQUID) rings locally coupled, unidirectionally as well as bidirectionally, in a ring configuration; it is well known that each individual SQUID can be biased through a saddle-node bifurcation to oscillatory behavior. Exploring parameter variations, such as; inductive coupling between neighboring elements, unconventional grating and fabrication parameters may also lead to significant performance enhancement. Applications of these devices include: geological equipment, biomedical such as MRI machines, and also, devices with the ability to detect and amplify resulting in a new generation of electrically small antennas.

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MS20

A Dynamical Systems Approach to Design and Operate Dynamic Sensors

A large class of dynamic sensors exhibit nonlinear input-output characteristics, often corresponding to a bistable potential energy function. Examples include: magnetic field sensors, e.g., fluxgate sensors, ferroelectric sensors, and mechanical sensors, e.g., acoustic transducers made with piezoelectric materials. Many of these sensors have assisted mankind in analyzing and controlling thousands of functions for many decades. As new technologies emerge, however, more powerful and more efficient sensors are required. Using ideas and methods from nonlinear dynamics research (in particular bifurcation theory) in Engineering, Mathematics, and Physics, we present theoretical and experimental results which demonstrate that higher sensitivity, lower power-consumption, and reduced costs, can all be achieved through an integrative approach that combines a novel Intelligent Magnetic Sensor (IMS) network architecture with a new read-out technique, the Residence Time Detection (RTD). The IMS/RTD concept is device-independent, so that similar principles can be readily adapted to a wide variety of sensors. In this minisymposium, we will consider, in particular, fluxgate magnetometers, Superconducting Quantum Interference Devices, and electric-field sensors.

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MS21

Solving Large-Scale Graph Optimization Problems on Massively-Multithreaded Machines

Massively multithreaded machines such as the old MTA-2 were designed to effectively solve latency-bounded computations: those with a large amount of communication relative to computation and little locality. These properties are a large part of the reason that graph algorithms are notoriously hard to parallelize. We will describe graph algorithms for massively-multithreaded architectures such as the new Cray XMT with a particular emphasis on algorithms that have applications to data mining for social networks.

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MS21

Recent Advances in Partitioning and Load-Balancing for Parallel Scientific Computing

To distribute data and work among processors such as to maintain load balance and also minimize communication is a challenging optimization problem. Highly specialized algorithms and software have been developed for this purpose to support large parallel computations. The CSCAPES SciDAC institute leads R&D in this area, e.g., the Zoltan load-balancing toolkit. We discuss recent developments related to Zoltan, and present advances in sparse matrix partitioning methods.

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MS21

Robust Optimization Methods for Combinatorial Optimization

Discrete models of large, complex systems like national infrastructures and complex logistics frameworks naturally incorporate many modeling uncertainties. Consequently, there is a clear need for optimization techniques that can robustly account for risks associated with modeling uncertainties. This talk will summarize progress in the analysis of solution robustness for large-scale applications. In particular, we consider scalability challenges for robust optimization in applications like water security and infrastructure planning.

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MS21

Low-memory Algorithms for Sensor Placement in Municipal Water Networks

Current state-of-the-art algorithms for designing early-warning sensor networks for municipal water network rely upon large numbers of simulations of potential contamination incidents. Sensor placement problems for full-size networks could require hundreds of GB of data from simulations. Yet the EPA and water utilities wish to design sensor networks using standard PCs. We will describe low-memory algorithms that can in practice provide provably optimal solutions to reasonable-sized problems on real networks.

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MS22

Inverse Problem in Seismic Imaging

This presentation concerns estimation of the sound speed inside the earth from time migration which is of great importance for the oil industry and earthquake analysis. We derive theoretical relationships and PDE's in 2D and 3D for the sound speed. We show that the problem is both sensitive and ill-posed. Nonetheless we develop numerical techniques that include finite difference schemes with small regularizing terms and efficient Dijkstra-like time-to-depth conversion algorithms solving this inverse problem.

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MS22

Velocity Extensions and the Level Set Method

We present an alternative way of doing velocity extensions for the level set method that more accurately represents the characteristics of the moving front. In addition to improving the level set method, it can also be used to do the fast marching method when the speed function is nonmonotonic and also to advance the level set method with a relaxed time step restriction.

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MS22

Linear Programming Interpretation of Perron's Method

Recently there has been a renewed interest in building solvers for nonlinear elliptic equations, such as the Monge-Ampere equation, the Pucci equations of stochastic control, and the Infinity Laplacian, among others. Up until now, the main effort has been on building convergent schemes, but the solvers have been slow. The challenge in building fast solvers for nonlinear equations is that due to the strong nonlinearity, linearization is ineffective. Instead, solvers are explicit and restricted by the nonlinear CFL condition, which gets increasingly stringent as the problem size grows. (Fast solvers for first order Hamilton-Jacobi equations have been built, but since they rely on a the method of characteristics, they can't be adapted to the second order case). The idea of this talk is to reformulate the solution of the PDE as a convex optimization problem, and then take advantage of existing solvers for optimization problems. The reformulation is accomplished via a small modification of Perron's method. When the PDE is of a special form, which includes the value of function of a stochastic control problem, we obtain a Linear Program (LP) for the solution. As a test of principle, in one dimension and two dimensions, for toy stochastic control problems, we obtain orders of magnitude speed up using commercial LP solvers. To make this tool of more general use, better (probably custom) LP solvers are needed. While in theory all convex equations can be written as a stochastic control problem, in practice this in not practical due to the large number of constraints. Finding good solvers for the general case is another open problem.

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MS22

Contraction Property of the Fast Sweeping Method

In this talk I will present a nice contraction property of the fast sweeping method. In particular, we will show that the contraction property plus right ordering will guarantee fast convergence for an iterative method. The contraction property will also imply global error control through a diffusion type of mechanism.

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MS23

Chasing $1,000,000: How We Won the Netflix Progress Prize

The collaborative filtering approach to recommender systems predicts user preferences for products or services by learning past user-item relationships. Their significant economic implications made collaborative filtering techniques play an important role at known e-tailers such as Amazon and Netflix. This field enjoyed a surge of interest since October 2006, when the Netflix Prize competition was commenced. Netflix released a dataset containing 100 million anonymous movie ratings and challenged the research community to develop algorithms that could beat the accuracy of its recommendation system, Cinematch. In this talk I will survey some of the principles and algoeirhms, which has led us to winning the 2007 Progress Prize in the Netflix competition.

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MS23

Global Positioning from Local Distances

In many applications, the main goal is to obtain a global low dimensional representation of the data, given some local noisy geometric constraints. In this talk we will show that problems in Cryo-Electron Microscopy for protein structuring, NMR spectroscopy for protein structuring, sensor networks and surface reconstruction can all be solved by constructing suitable operators on their data followed by the computation of a few eigenvectors of sparse matrices corresponding to the data operators.

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MS23

Combinatorial Hodge Theory and a Geometric Approach to Ranking

Modern ranking data are often incomplete, unbalanced, and arise from a complex network. We will propose a novel approach to analyze such data from the perspective of combinatorial geometry and topology, using combinatorial Hodge theory as our scalpel. In this framework, ranking data is represented as flows on a graph and Hodge-decomposed into three orthogonal components that are globally consistent, locally consistent, and locally inconsistent respectively. Rank aggregation then naturally emerges as projections onto a suitable subspace and an inconsistency measure of the ranking data also arises as curl distributions.

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MS23

Variable Selection: Tractable Upper Bounds on the Restricted Isometry Constant

We use recent semidefinite relaxation results to produce tractable upper bounds on sparse eigenvalues. We then test the performance of these bounds on various random matrices from compressed sensing, for which asymptotic estimates are known.

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MS24

Frequency Encoding of Steady Inputs in Neuronal Competition Models

We investigate a class of firing rate models that describe alternating rhythmic phenomena that arise in several neural contexts including motor coordination and perception of ambiguous sensory stimuli. These models rely on mutual inhibition and a slow process (such as adaptation or synaptic depression) and they all show nonmonotonic dependency of the oscillations' frequency on the stimulus strength. We demonstrate that two mechanisms (acting in specific ranges of input) are responsible for the observed dynamics.

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MS24

A Selection of Models Linking Endogenous DNA Damage to the Developmental Origins of Neuronal Genetic Variability

The operation of neuronal circuitry within human brain, involving $10^{1}4$ synaptic connections between $10^{1}1$ neurons, relies on genetic and proteomic variability at a single-neuron level—mosaicism—to make possible the precise specification of each individual synapse. We will present mathematical modeling that, in its most complex form, incorporates single-cell level gene-regulatory networks within structured branching point processes to describe the kinetics of genetically-diverse populations of neural progenitor cells (NPCs). We discuss simplifications of this framework, and comparisons of selected models, within the context of prevailing questions about the nature and developmental origins of neuronal variability.

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MS24

Connections Between Axonal Transport, Cell Metabolism, and Neuronal Network Function in Health and Disease

The transport of materials in nerve axons gives rise to systems of reaction-hyperbolic PDEs studied by the speaker and by A. Friedman. Recent experimental evidence suggests strongly, however, that metabolism in the axons also depends on transport to and from neighboring glial cells and disruptions in either transport system plays an important role in network dysfunction and neurodegenerative diseases. New mathematical models linking axonal transport and glial function to neuronal health will be presented.

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MS24

Indirect Detection of Spill-over: A Synthesis of Experiment and Modeling to Determine the Time Course of Neurotransmitter in the Synaptic Cleft

The connectivity of neurons in the hippocampus depends in part on whether neurotransmitter from one release site can leak out and activate receptors in another synapse or extrasynaptic patch. The existence of such "spillover" is under debate in the neuroscience community, since measurements of neurotransmitter in such detail cannot, as of yet, be made. Experimental evidence of spillover is thus indirect, and our modeling provides a critical link in the analysis of this phenomenon.

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MS25

Super-Grid-Scale Models as Absorbing Layers for the Navier-Stokes Equations and Other Applications

We discuss further developments to the super-grid-scale model, an absorbing layer technique for conservation laws on infinite and semi-infinite domains. The model exploits connections between sub-grid-scale models for filtered equations (e.g. turbulence models) and closures for large-scale motions that are unresolved when the equations are windowed. Here we examine in greater detail the reflectivity of these layers to linear waves, and examine new super-grid closures that reduce reflectivity.

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MS25

Complete Plane Wave Expansions and Optimal Radiation Boundary Conditions

We develop expansions of the solution of the time-dependent wave equation in a half-space in terms of plane waves which both propagate and decay. Local radiation boundary condition sequences are then devised which are uniformly accurate when applied to this exact representation, leading to geometrically flexible conditions satisfying optimal complexity estimates. Numerical experiments are presented which demonstrate the efficiency of the new conditions. We also discuss their implications for optimizing discrete PMLs.

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MS25

Discrete and Energy-Absorbing Far-Field Boundary Conditions for a Finite Difference Approximation of the Elastic Wave Equation

We will show example computations of seismic wave propagation with first order Clayton-Engquist far-field boundary conditions, that demonstrate that the stability of these conditions is conditional on a low c_p to c_s ratio. We will derive a new Clayton-Engquist-like boundary condition that is guaranteed to be energy absorbing for any ratio of c_p to c_s. We will prove this also for the fully discretized problem.

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MS25

Stable Outgoing Wave Filters for Anisotropic Waves

In this talk I present a new type of open boundary conditions, the phase space filter. Based on modern scattering theory, the basic idea is to identify in phase space the region corresponding to outgoing waves and filter them before they reach the computational boundary. I'll discuss Schrodinger, (Anisotropic) Maxwell and Molecular Dynamics models. The method is stable for all linear waves. It is local in time and pseudo-local in space, and imposes few restrictions on the interior solver and coordinate system. This is a joint work with Avy Soffer.

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MS26

Multirate SSP Methods for Hyperbolic PDEs

A set of explicit multirate time discretization methods based on multistep methods and partitioned Runge-Kutta is presented for hyperbolic conservation laws. It allows different timesteps to be used in different parts of the spatial domain, while being second order accurate in time and conservative. Linear and nonlinear stability are guaranteed only under local CFL conditions. The necessity to take small global timesteps restricted by the largest CFL number is thus avoided. Numerical experiments for the advection and Burgers' equations confirm the theoretical results.

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MS26

High Order Discretizations of Kinetic Equations

In this talk we present some recent developments on the construction of high-order schemes for kinetic equations. Applications to BGK-type equations are presented and discussed.

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MS26

Do We Know WENO?

We discuss the linear stability of several popular combinations of the fifth-order weighted essentially non-oscillatory (WENO5) method with time integration methods for numerically integrating hyperbolic conservation laws. We find that a sufficient condition for the combination of an explicit Runge-Kutta (ERK) method and WENO5 to be linearly stable is that the linear stability region of the ERK method should include the part of the imaginary axis of the form $[-i\mu, i\mu]$, for some $\mu > 0$.

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MS27

Student Research Interships at the National Laboratories

I will describe some of the National Laboratory summer programs for academically strong students in science and engineering. These programs are designed to give the students hands-on research experience in developing and analyzing advanced mathematical models as well as access to the extensive scientific computing resources.

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MS27

An International Research Experience for Undergraduates in Numerical Analysis and Scientific Computing

In our current global society, it is essential that mathematics students receive an education that prepares them for research with cultures beyond their own. This presentation discusses an international NSF Research Experiences for Undergraduates program, focusing on numerical analysis and scientific computing with applications in applied science and engineering, in which students engage in research with faculty at Hong Kong universities. The presentation includes a discussion of the projects undertaken by the students as well as the outcomes to date.

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MS27

Teaching Computational Science and Engineering

This talk describes a modern course on computational methods for engineers and scientists and applied mathematicians (seniors/beginning graduates). The structure of the course has evolved from teaching 18.085 at MIT for 20 years. The original text Introduction to Applied Mathematics is now replaced by the new text Computational Science and Engineering (CSE). The author hopes that others will want to move away from ancient formula-based courses toward this solution-based course.

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MS27

SIAM Undergraduate Research Online

This new online publication has recently been announced by SIAM. The speaker is the first Editor in Chief and will describe the publication and its role within undergraduate research opportunities. This publication not only provides an excellent outlet for undergraduate research, it also provides faculty who are recruiting graduate students with particular strengths a natural resource for identifying potential research assistants.

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MS27

Undergraduate Research in Image Processing

Image processing is an ideal research area for undergraduate applied math students, as students can get started quickly with limited programming experience and can see visual results rather quickly. I will discuss my experience working with UCLA math majors on research projects in image processing. Specifically, I have worked with students on processing high-dimensional hyperspectral data sets. I will also touch on the problems in hyperspectral imaging and suggest areas to explore.

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MS28

Nonlinear Optimal Control Tracking and Parameter Estimation Through Dynamical Coupling

By dynamical coupling of data with known models, we determine underlying parameters and unmeasured state variables for a variety of systems, including Lorenz, Colpitts, and Hodgkin-Huxley neurons. The dynamic coupling is mediated by use of a cost function, which is minimized by optimization software to achieve the desired synchronization.

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MS28

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS28

POD Model Reduction of Large Scale Geophysical Models

4DVAR is a powerful tool for data assimilation in meteorology and oceanography. A major hurdle in use of 4DVAR for realistic models is dimension of control space ,generally equal to size of model state variable and typically of order $10^7 - 10^8$ and high computational cost in computing cost function and gradient requiring integration of model and adjoint. This led to introduction of a reduced model approach of POD type by projecting the full model dynamics into reduced space. Experience with a large-scale POD-based reduced model and adjoint for unstructured ocean model, 3-D finite element Imperial College Ocean Model (ICOM) including adaptive mesh capability is presented along with work on a ocean reduced gravity model. An approach using 4-D VAR data assimilation with reduced order POD model will be outlined.

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MS28

Adaptive Observation of Contaminant Plume, Hurricane, and Ocean Systems

Two new algorithms for Adaptive Observation are presented. 1) The first algorithm discussed is based on the application of model predictive control (MPC) theory to minimize a very targetted objective: specifically, a quantification of the estimate uncertainty at the forecast time. This estimate uncertainty, in turn, is quantified using the EnKF procedure by marching the ensemble forward to the forecast time while assimilating the anticipated measurements along the candidate sensor trajectories. This algorithm is applied to optimize the trajectories of several sensor-equipped UAVs in an atmospheric contaminant plume forecasting problem. 2) The second algorithm discussed is again based on the application of MPC theory in order to now uniformly distribute hundreds or even thousands of underactuated sensor-equipped vehicles in known velocity fields. This algorithm is applied to two specific applications: a) optimization of the vertical motion of sensor-equipped balloons (that is, buoyancy-controlled "sondes") in order to achieve pseudo-volume-filling sampling (PVS) within a hurricane, and b) optimization of the vertical motion of sensor-equipped submersibles (that is, buoyancy-controlled "floats") in order to achieve PVS over the oceans of the earth in the Argo project.

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MS29

High Order Numerical Schemes for Non-Conservative Hyperbolic Equations. Applications to Geophysical Flows

This work is concerned with the development of well-balanced high order finite volume schemes for two-dimensional nonconservative hyperbolic systems. In particular, we are interested in extending the methods introduced in Castro-Gallardo-Pares (2006) to the two-dimensional case. We also investigate the well-balance properties. We focus in applications to some geophsical flows.

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MS29

New Savage-Hutter Models for Submarine Avalanches

We present a new two-layers model of Savage-Hutter type to study submarine avalanches. A layer composed of fluidized granular material is assumed to flow within an upper layer composed of a non-viscous fluid. The model verifies an entropy inequality and preserves water at rest for a sediment layer for smaller angles than the angle of repose of the material. The model can be used to simulate some type of tsunamis.

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MS29

Inclusion of Non-Hydrostatic Pressure in Numerical Schemes for Free-Surface Gravity Flows

The shallow water equations present the advantage to modelers of using two-dimensional depth averaged equations to describe the horizontal extent of many geophysical flows, without having to resolve vertical variation within the flow. This reduces the cost and complexity of numerical methods. However, the shallow water equations are based on a hydrostatic pressure assumption, which is often poorly satisfied by flows, even very shallow ones, over rapidly varying topography—a feature which characterizes most debris flows. I will discuss the incorporation of nonhydrostatic terms into depth-averaged equations, similar to the shallow water equations, some of the resulting numerical challenges that arise, and some solutions to these challenges.

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MS30

A How Can I Say that A Toy Model Reminds Me of My Observations? Modeling and Comparing Non-Conjugate Systems– Mostly Conjugate

We address a fundamental modeling issue in science as related to the field of dynamical systems: when is a model of a physical system a good representation? Conjugacy provides a means to define if two systems are dynamically equivalent; it is the central equivalence relationship in the field of dynamical systems. However, it cannot cope with systems which are not dynamically identical. We develop mathematical technology to decide when dynamics of a toy model are like dynamics of the physical system, since the concept of conjugacy is too rigid for such cases.

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MS30

Applied Dynamics for Weather and Climate Prediction

Complex spatiotemporal dynamical systems often exhibit comparatively low-dimensional behavior, at least over reasonably short time scales, despite the high dimension of the phase space. This behavior has been exploited to yield a fast, accurate scheme to estimate initial conditions (say of the atmosphere) from noisy measurements. I will discuss recent work with collaborators at the University of Maryland to combine measurements and forecasts to estimate certain types of errors in the dynamical models themselves.

Potential applications to weather and climate forecasting will be described.

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MS30

Inferring Network Dynamics from Time Series

Problems of reconstructing dynamical information from network observations are discussed. For networks with unknown topology, time series data from nodes can be used to infer network links. We present an algorithm especially suited for sparsely-connected networks that has low data requirements. For networks with known topology, we investigate methods for reconstructing dynamics at individual nodes.

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MS30

Chain Recurrence Rates

We investigate the properties of chain recurrent, chain transitive, and chain mixing maps (generalizations of the well-known notions of non-wandering, topological transitivity, and topological mixing). We describe the structure of chain transitive maps. These notions of recurrence are defined using ϵ-chains, and the minimal lengths of these ϵ-chains give a way to measure recurrence time (chain recurrence and chain mixing times). We give upper and lower bounds for these recurrence times and relate the chain mixing time to topological entropy.

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MS31

Dynamics of Closely Coupled Nephrons

A human kidney contains approximately one million nephrons, the basic functional unit that filters blood into urine. The functional state of a nephron in a normotensive rat is experimentally characterized as either steady or as limit-cycle oscillations (LCO). The oscillatory behaviors in nephrons flows are mediated by a negative feedback system known as tubuloglomerular feedback (TGF). Although the physiological significance of LCO still remains unclear, based on experiments it is suggested that LCO may act to enhances the sodium chloride excretion and thereby limit the degree of hypertension. It is known that many mathematical models of control exhibit oscillatory solutions; oscillations are also a feature of delay differential (or integral) equations. In this talk we present the modeling of nephrons with these mathematical tools and interpret the results analytically using bifurcation analysis and numerically by using computer simulations.

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MS31

Analysis of Stability and Dispersion in a Finite Element Method for Debye and Lorentz Dispersive Media

In this talk we discuss the stability properties and the phase error of a finite element scheme for Maxwell's equations coupled with a Debye or Lorentz polarization model for modeling wave propagation in dispersive media. We present numerical simulations which validate our analytical results and determine a practical guideline for the choice of discretization parameters. We also compare this method with finite difference methods that have been analyzed in the literature.

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MS31

On the Stability Analysis of Wavefronts in Marginal Cases

On the example of wavefronts supported by the high Lewis number combustion model I discuss various issues in the stability analysis that arise at both the linear and nonlinear level. In particular, I discuss how the Stability Index Bundles are used to relate the spectra of wavefronts with sufficiently high Lewis numbers to the limiting, infinite Lewis number case (joint work with Chris Jones). I also present a technique for proving nonlinear stability of the front, in a weighted norm, when the spectral information is not definitive.

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MS31

Effects of Local Coupling on Asynchronous Solution of the Kuramoto Model

We investigate the effects of introducing local coupling between groups in a network of noisy Kuramoto oscillators in m groups. We study the stability of the asynchronous state by using the probability density approach. There is a critical value for the local coupling that disrupts the asynchronous solution. This couplingstrength depends on the interplay between the coupling functions and the noise strength. We also did simulations that validate our analytical findings.

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MS32

Regularity and Synchrony for Motor Proteins

The majority of intracellular transport is performed by a family of nanometer-scale proteins typically known as "motor proteins". These motors convert chemical energy to mechanical work, but, unlike macroscopic motors, the energy is transferred by a single ATP molecule. Thus one expects the dynamics of the motor to be quite random; however, it has been observed that populations of such motors act regularly in certain situations. We present an analysis of several motor protein models and show that there are generic organizing principles which can lead to regular behavior in a motor's dynamics. This analysis is able to explain observations made in the literature of regularity for myosin V during vesicle transport and myosin II during muscle contraction.

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MS32

Homogenization-Based Approach for Coarse-Graining Molecular Motor Models

Homogenization theory provides a framework for computing effective properties of stochastic (Brownian) molecular motor models in terms of their design parameters. We present a spectral numerical scheme for solving these equations and apply it to examine themes such as continuous-in-time modulation of a flashing ratchet and the validity of approximating continuous motor models by simpler discrete random walk models.

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MS32

Coordinated Dynein Motility: Long Runs vs. High Speed

The processive stepping of dimeric motor proteins requires not only the coordination of the biochemical and mechanical cycles of the individual heads, but also coordination between the two heads. Using kinetic data for individual heads, we systematically explore the possible mechanochemical cycles for double-headed dynein. In all cases, we determine necessary conditions for reproducing both the high processivity and high motor velocities measured experimentally. Finally we discuss possible biophysical mechanisms for such coordination.

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MS33

Challenges of Nuclear Calculation: an Introduction to Mathematicians

There is now a strong consensus in the nuclear engineering community that a strategy relying on the development of advanced modeling and computational techniques will be essential for obtaining high fidelity simulation of future nuclear reactor systems. The state-of-the-art of nuclear calculations, based on the multi-level homogenization theory approach, suffers from two fundamental deficiencies: a) lack of mathematical theoretical analysis to assess the accuracy of the solution due to the various homogenization assumptions, and b) the inefficient communication between the different scales and physics involved in the simulation. This talk will introduce the state-of-the-art of nuclear calculations, especially in view of their limitations, to the applied mathematicians and computational scientists community. The objective is to develop a channel of communication between the nuclear and mathematical community that can help promote more promising approaches to overcome the limits of current nuclear analysis and design methods.

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MS33

A Diffuse Interface Model for Electrowetting Drops In a Hele-Shaw Cell

Electrowetting has recently been explored as a mechanism for moving small amounts of fluids in confined spaces. We propose a diffuse interface model for drop motion, due to electrowetting, in a Hele-Shaw geometry. In the limit of small interface thickness, asymptotic analysis shows the model is equivalent to Hele-Shaw flow with a voltage-modified Young-Laplace boundary condition on the free surface. We show that details of the contact angle significantly affect the timescale of motion in the model. We measure receding and advancing contact angles in the experiments and derive their influences through a reduced order model. These measurements suggest a range of timescales in the Hele-Shaw model which include those observed in the experiment. The shape dynamics and topology changes in the model agree well with the experiment, down to the length scale of the diuse interface thickness.

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MS33

Parallel Coupling of Earth Science Models with ESMF

We present results from the Earth Science Modeling Framework, a coupling framework for Earth Science models. We use the Parallel-Rendezvous approach of Stewart et al. to generate weight matrices for bilinear and conservative interpolation operators, in parallel. The parallel algorithm allows for more timely weight generation, and is able to handle larger coupling problems without memory issues, compared to standard weight generation tools used currently in the community. A new interpolation approach using patch recovery is used to generate smoothing interpolation operators for coarse to fine grid scenarios. This approach is investigated in the context of a coupled atmospheric/ocean model.

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MS34

Recent Development of High Order WENO-Z Finite Difference Methods

A generalization of the smoothness indicators of WENO scheme of arbitrary order will be presented. Some interesting properties and structures of the resulting smoothness indicator influence matrix, which resulted in a compact formulation of the smoothness indicators of arbitrary order, will be discussed. The new improved high order WENO-Z finite difference scheme based on high order information within the compact stencils are derived and its applications for multi-dimensional hyperbolic conservation laws will be presented.

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MS34

A Full Vectorial Generalized Discontinuous Galerkin Beam Propagation Method (GDG-BPM) for Nonsmooth Electromagnetic Fields in Waveguides

In this talk, to accurately handle the discontinuities of electromagnetic fields in inhomogeneous optical waveguides, we propose a generalized discontinuous Galerkin beam propagation method (GDG-BPM) by combining beam propagation method with a newly developed generalized discontinuous Galerkin method [J. Comput. Phys. 227 (2008) 2387-2410], which uses distributional variables to account for jumps across material interfaces. Numerical results validate the high order accuracy and the exibility of the method for various types of interface conditions.

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MS34

A WENO/Radial Basis Function Hybrid Method for Solution of Hyperbolic Time Dependent PDEs

Hybrid high order methods have been developed to deal with discontinuous solutions based on the hybridization of spectral and WENO methods. For the spectral-WENO hybrid method, the additional interpolation step is necessary due to the inconsistency of grids. To efficiently deal with the grid inconsistency and avoid the interpolation steps, the RBF-WENO method is developed. The mesh-less properties of the RBF method yields more efficient algorithm. Numerical examples will be presented to verify the efficiency of the method.

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MS34

An Iterative Adaptive Multi-Quadric Radial Basis Function Method for the Detection of Local Jump Discontinuities

A new edge detection method is developed using multiquadric radial basis functions. We show that the global maximum of the expansion coefficients exists at the strongest jump. Furthermore its growth rate is exponential but becomes linear if the corresponding shape parameters vanish. Upon vanishing shape parameters, the global maximum exists now at the next strongest jump. Repeating this procedure yields the successive detection of edges. Numerical examples will be given from images and PDEs.

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MS35

Coarse-Grained Modeling and Simulation of Lipid Bilayer Membranes

Lipid molecules consist of a hydrophilic head group and a hydrophobic tail whose competition leads to intriguing phases. These include micelles, bilayered fluidic sheets, or enclosed vesicles with rich geometric structures having features over a wide range of length-scales. A fundamental challenge in studying lipid systems is to understand how molecular level interactions lead to observed large-scale phenomena. In this talk we shall discuss a coarse-grained modeling and simulation approach which captures many of the features of lipid bilayers. We shall then discuss hydrodynamic phenomena related to bilayer membranes. In particular, the role of thermal fluctuations and the coupling of membrane deformations and lipid flow. We will also discuss the role of fluid-like features of the membrane in the dynamic coupling of protein inclusions within a bilayer.

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Frank Brown

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MS35

Physics of Viral Entry

A stochastic model is developed to describe viral entry mechanisms. Enveloped viruses can enter a cell through endocytosis or membrane fusion. Which process is more likely to occur depends on physical conditions such as pH. In our analysis, we consider one and two-receptor engagement models and determine the range of parameters in which each entry pathway is favored.

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MS35

Interaction of Vesicle Membrane with Fluid and Substrate

In this talk, we present some recent works on the modeling and simulations of vesicle membranes and their interaction with background fluid and curved substrate. Our studies are based on the classical Helfrich bending elasticity model, with extensions to incorporate the effect of the fluid transport and the adhesion of the substrate respectively. We also discuss how these problems can be studied effectively using a phase field diffuse interface formulation.

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MS35

Surface Phase Separation and Flow in Vesicle Biomembranes

Vesicle membranes usually have bilayer structures composed by lipid molecules with hydrophilic heads and hydrophobic. In an aqueous environment, they form vesicles and exhibit rich shape transition behaviors because of their highly flexible structures. Physical processes like phase separation are usually coupled with morphology changes in membranes. Because of the presence of high-order nonlinear terms in these physical processes, it is highly challenging to simulate the shape transition and phase decomposition on a moving surface. Here we present a mathematical model describing the nonlinear coupling among the flow, vesicle morphology and the evolution of the surface phases. We solve the fluid field using Boundary Integral Method and Immersed Boundary method. We use a nonstiff algorithm to solve the Cahn-Hilliard type material field on the vesicle boundary. Numerical results show detailed dynamics of phase separation and shape transformation.

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MS36

Software for Parallel Adaptive Methods

The PLTMG software package solved a variety of parameter dependent, nonlinear PDES, obstacle problems and optimal control problems in general regions of the plane. The software uses Lagrange triangular finite elements of order $1 \leq p \leq 3$, and features several adaptive meshing options, algebraic multilevel iteration for solving linear systems of equations, and optimization strategies to address nonlinearities, parameter dependence, obstacles, etc. The package implements the Bank-Holst strategy for parallel adaptive computation.

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MS36

Writing a General Purpose Finite Element Library - Deal.II

An overview of the software design and data abstraction decisions chosen for deal.II, a general-purpose finite element library written in C++, is given. The library uses advanced object-oriented and data encapsulation techniques to break finite element implementations into smaller blocks that can be arranged to fit users requirements. Through this approach, deal.II supports a large number of different applications covering a wide range of scientific areas, programming methodologies, and application-specific algorithms, without imposing a rigid framework into which they have to fit. A judicious use of programming techniques allows us to avoid the computational costs frequently associated with abstract object-oriented class libraries. A detailed description of the abstractions chosen for defining geometric information of meshes and the handling of degrees of freedom associated with finite element spaces, as well as of linear algebra, input/output capabilities and of interfaces to other software, such as visualization tools, will be presented.

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MS36

Application of a Parallel Adaptive Finite Element Code to Confined Interacting Atoms

PHAML is a Fortran 90 module for the solution of 2D elliptic boundary value or eigenvalue problems. It features adaptive grid refinement (h, p or hp), multigrid solution, message passing parallelism, and extensive visualization. We will describe the design of PHAML and its application to the solution of a Schrödinger equation that models two interacting atoms in an optical trap. This application has very strong local behavior that requires adaptive refinement with high order elements.

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MS36

Finite Element Software for Petascale Systems

The HHG and ParEXPDE programs have been developed as software frameworks for finite element computations on future PetaScale systems. They use multilevel solvers and carefully designed data structures together with a user-friendly programming interface that can hide the complex architecture-aware parallel implementation. On the SGI Altix we demonstrate scalability experiments for FE systems with up to 10 000 compute cores and in excess of 300 000 000 000 unknowns, using close to 40 TByte of memory.

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MS37

Iterative Algorithm for Wave Functions Optimization in Density Functional Theory: Inexact Newton with Anderson Acceleration

We describe a numerical algorithm to solve electronic structure problems in Density Functional Theory. The approach can be seen as a subspace accelerated inexact Newton solver for the non-linear Kohn-Sham equations. It is related to a class of iterative algorithms known as DIIS in the electronic structure community. The method is illustrated with examples of real applications using a finite difference discretization and multigrid preconditioning.

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MS37

Exposing More Parallelism in Quantum Chemistry Applications: Moving Beyond the MPI and Hybrid MPI/Multithreaded Programming Models

Current approaches to the parallelization of quantum chemistry algorithms entails partitioning the problem into distinct steps and selecting a an associated level of granularity for each of these steps. This approach has flaws that increase the difficulty of getting good efficiency at large scales and reduces the ability to map the problem to the deep memory hierarchies in modern parallel machines. This talk will discuss alternative parallelization strategies and the implication for efficiency of quantum chemistry algorithms.

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MS37

A Trust Region Direct Constrained Minimization Method for Electronic Structure Calculations

Density functional theory (DFT) is the most widely used ab initio method in material simulations. At the heart of many DFT codes, one typically finds a Self Consistent Field (SCF) iteration for solving the Kohn-Sham equations. In this talk, I will discuss an alternative approach based on a trust region optimization method that directly minimizes the Kohn-Sham total energy directly. Numerical experiments demonstrate that this approach is more efficient and robust than SCF.

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MS37

Chebyshev-Filtered Subspace Iteration Method for Density Functional Theory Calculations

We present a Chebyshev-Filtered Subspace Iteration (CheFSI) method for Density-functional theory (DFT) calculations. The CheFSI method replaces the expensive eigenvector calculations by directly filtering the basis of the desired eigensubspace using adaptive Chebyshev polynomials. Approximate eigenvectors are computed only at the first self-consistent-field (SCF) iteration, latter SCF steps no longer compute eigenvectors. Avoiding the expensive eigenvector calculations leads to significant speedup in SCF calculations over iterative eigensolver-based approaches. CheFSI method enables us to perform a class of highly challenging DFT calculations that were not feasible via eigensolver-based approaches.

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MS38

Parameter Selection Techniques for Projection-based Regularization Methods

In hybrid regularization methods, regularization is applied to a smaller, projected version of the large-scale discrete ill-posed problem to compute a regularized solution to the original problem. The challenge is computing regularization parameters efficiently for the projected problem, viewed in the context of the original problem. We discuss options for computing one or two parameters when Tikhonov regularization is employed. As an application for the two parameter case, we consider image reconstruction in parallel MRI.

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MS38

The Chi-squared Method for Parameter Estimation, Combining Data Sets and Uncertainty Quantification

We will describe the chi-squared curve method for parameter estimation recently developed by Mead (2007) and Mead and Renaut (submitted). The chi-squared curve method is considerably more efficient, and as accurate as traditional L-curve and cross-correlation methods for parameter estimation. This method involves forming a maximum likelihood estimation problem, and here we will include soil moisture and pressure head data from both insitu, and laboratory core measurements. We assume all data contain errors, thus this method does not calibrate a model with data, rather parameter estimates are found within a priori data uncertainty ranges.

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MS38
Improving the Efficiency of the Chi-squared Regularization Method for Large Scale Regularized Least Squares

Recently, Mead showed that a statistical result on the χ^2-distribution of the Tikhonov regularized least squares (RLS) cost functional can be used for estimating an optimal regularizing parameter. A Newton algorithm based on the Generalized Singular Value Decomposition (GSVD) gives a convergent algorithm for the parameter and RLS solution. Here I present an efficient implementation avoiding the GSVD, and making the technique feasible for large scale RLS using the LSQR algorithm for calculation of the successive iterative solutions.

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MS38
Regularization by Residual Periodograms

After an ill-posed problem is transformed to have independently, identically $n(0, 1)$ data errors, the distribution of the residuals for an estimate can be compared with the expected error distribution. We treat the residuals as a time series and choose the regularization parameter to make their distribution approximate that of normally distributed white noise. We develop and evaluate a method which uses the cumulative periodogram of the residuals to guide that choice.

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MS39
The Internet's Router-Level Topology: Principles, Models, and Validation

The Internet is a complex conglomeration of competing networks that are owned and operated by Internet Service Providers (ISPs) who must balance the technological capabilities of their networks with the economic drivers of their business. We present a first-principles approach to modeling router-level connectivity that focuses on the causal forces at work in network design and aims at identifying the economic and technical drivers responsible for the observed large-scale network behavior.

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MS39
Online Social Networks - Connecting People like Never Before

Social networking services are a fast-growing business in the Internet. These online servies offer an unprecedented opportunity for social scientists and computer scientsts alike to capture and decipher human interactions and design systems to facilitate such interactions. We begin this talk with a comparison of topological structures from major online social networking services, namely, Cyworld, MySpace, and orkut. Each of them has more than 10 million users and has been a dominant player in respective markets. We analyze the degree distirubtions, clustering coefficients, degree correlations, and average path lengths. Except for Cyworld, we do not have access to the complete topology, and resort to sampling for the other networks. We review briefly the sampling techniques employed in the measurement effort. As online social networking services have become the budding ground for cyber communication, their topological structures attest to the existence of cyber-only relationships. However, the online friendship is only a declaration of relationship. Actual interaction could be vastly different from one relationship to another. We compare the topological structure against the networks built from actual interaction, more specifically, guestbook comments in the Cyworld. We believe this work marks only the beginning of interdisciplinary study in social science, economics, mathematics, and computer science. We conclude this talk with ongoing research in related fields.

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MS39
On the Internet's AS-level Topology

Despite significant efforts to obtain an accurate picture of the Internet's actual connectivity structure at the level of individual autonomous systems (ASes), much has remained unknown in terms of the quality of the inferred AS maps that have been widely used by the research community. We assess the quality of the inferred Internet maps through case studies of a set of ASes. These case studies allow us to establish the ground truth of AS-level Internet connectivity between the set of ASes and their directly connected neighbors. They also enable a direct comparison between the ground truth and inferred topology maps and yield new insights into questions such as which parts of the actual topology are adequately captured by the inferred maps, and which parts are missing and why. This information is critical in assessing for what kinds of real-world networking problems the use of currently inferred AS maps or proposed AS topology models are, or are not, appropriate. More importantly, our newly gained insights also point to new directions towards building realistic and economically viable Internet topology maps.

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MS39

Empirical Characterizations of P2P Systems

During recent years, the pervasive deployment of Peer-to-Peer (P2P) systems had a profound impact on the Internet that is even more tangible than the impact of the Web. Ease of deployment and self-scaling are two key factors that continue to fuel the growing popularity of the P2P communication paradigm for a wide spectrum of large scale commercial systems ranging from content distribution to Internet telephony (e.g. Skype) and Internet TV. Despite the importance of the P2P communication paradigm and the far reaching impact of P2P systems on the Internet, fundamental properties and in particular the dynamics of large scale P2P systems are not well understood. This talk will focus on the IonP2P project whose goal is the investigation and development of new measurement and modeling methodologies to understand and accurately characterize properties and dynamics of large scale P2P systems.

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MS40

A Non-Smoluchowski-Type Model in the Coagulation-Fragmentation Kinetics

Smoluchowski approach in coagulation is based on binary collisions. However, experiments in, say, atmospheric clouds demonstrate that the interacting droplets are split in several parts. In 1999 a corresponding coagulation model was derived, whose solution is extremely close to the solution of the Smoluchowski equation. This explains why the Smoluchowski model can be well applied to the description of many processes even though they may have another base. In this talk we use our approach of 1999 to derive and analyze a new fragmentation model.

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MS40

Boundary Value Problems for Boltzmann Poisson Systems

We investigate the well posedness of stationary Vlasov-Boltzmann equations both in the simpler case of linear problem with a space varying force field, and, the nonlinear Vlasov-Poisson-Boltzmann system. For the former we obtain existence-uniqueness results for arbitrarily large integrable boundary data and justify further a priori estimates. For the later the boundary data needs to satisfy an entropy condition guaranteeing classical statistical equilibrium at the boundary. This stationary problem relates to the existence of phase transitions associated with slab geometries.

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MS40

Simulation of Mesoscopic Models for Self-Organization in Materials

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

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MS40

On Kinetic Equations of the Weak Turbulence Theory

Not available at time of publication.

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MS41

Second Order Necessary Conditions in Nonsmooth Optimization

We are concerned with the following optimization problem

$$F(\bar{x}) = \text{Local Minimum}\, F(x), \text{ subject to } x \in D, \qquad (P)$$

where X is a real Banach space of norm $||\cdot||$, $F : X \to IR$, IR the set of reals, and $D \subseteq X$, $D \neq \emptyset$. We establish some second order necessary conditions by means of the first and second order upper generalized derivatives of the nonsmooth objective function F. Our second order optimality conditions are formulated in terms of the Pavel and Ursescu's tangent vectors to D at $\bar{x}$. We describe the second order tangent cones to a set of the form $D_G = \{x \in X,\ G(x) \geq 0,\ G : X \to IR^m\}$, under appropriate assumptions on G. We analyze an example to illustrate the applicability of our results.

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MS41

An Extended Cutting Plane Method for a Class of Nonconvex Problems

We present a cutting plane method for a problem with a convex set constraint and a pseudo-convex objective function. We apply the method to a mathematical programming problem involving pseudo-convex functions.

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MS41

Slow Decay of Correlations of Chaotic Billiards

Billiard are popular models in statistical mechanics. Singularities in billiards lead to an unpleasant fragmentation of phase space. We obtained a very general and powerful method for estimating the polynomial decay rate of correlations for general nonuniformly hyperbolic systems with SRB measures. We applied the above method to several classes of billiards. Furthermore, to cover a larger class of billiards, we reproved exponential decay of correlations for reduced map by using coupling method.

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MS41

Fast 2–D Spline Interpolation Algorithm

Cubic splines are generally useful for interpolating grid-based data. I discovered that the standard methods for solving N x M spline system do not take advantage of its spline-specific format. An alternative approach for pre-computing coefficients and inverting the derivative matrix is presented. I confirm analytically and numerically that for large number of data points in each dimension (N ¿ 200), the new method is more than 3 times faster than the standard algorithm and is just as accurate.

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MS42

Modeling of Hurricane Storm Surges Driven by Winds and Waves

Studying coastal inundation due to hurricanes is of critical importance to the United States. Critical decisions will be made in the next several years on how to design better protection systems and improve emergency management practices in the event of future storms. Storm surge is caused by wind, atmospheric pressure gradients, tides, river flow, short-crested wind-waves, and rainfall. In this talk, we will discuss accurate numerical models which account for these effects.

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MS42

The Coupling of Viscoelastic Stresses and Biochemistry in the Lung

Airway surface liquids line lung pathways, trapping all the debris that comes in with inhaled air. These liquids, most famously "mucus", are transported by coordinated cilia, cough and tidal breathing toward the larynx where they are swallowed. Cells along the pathway are responsible for regulating biochemical release rates (e.g., of ATP), which affect ion channels, which govern water passage across the membrane. Other cells produce and release the mucin macromolecules that replenish the mucus layer. Experiments clearly show release rates are sensitive to mechanical stresses, which are transmitted from the airway surface liquids. This lecture will cover the status of our attempts to model the feedback among viscoelastic stresses, material properties, water volume, and biochemical concentrations.

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MS42

Multiphysics Issues in Computational Nuclear Engineering

Coupled physics phenomena are ubiquitous in nuclear power reactors. Such multiphysics problems frequently contain multiple time scales and length scales. Examples include thermo-mechanical behavior of a fuel rod, thermal-fluid neutronics behavior in the core, and the coupling of the core to the primary coolant system. In this presentation we provide some examples of state of the practice in each of these areas, along with analysis of some issues. Then we present evolving algorithmic approaches for overcoming understood shortfalls in the state of the practice.

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MS42

Current Approaches to Multiscale and Multiphysics Problems in Weather and Climate

Phenomena on micron scales have impact on planetary scale weather and climate through the physical processes of clouds, precipitation and radiation and the nonlinear advective processes which link disparate scales. In global computational models of the atmosphere all processes which are beyond the resolution of the numerical model are accounted for through the incorporation of process models or parameterizations. Traditionally, these process models are deterministic and empirical. Recently, there has been interest in moving towards a more proper stochastic treatment of of the problem of parameterization of physical process in large scale numerical models. The status of stochastic methodologies and the range of their possible atmospheric applications will be examined and contrasted to deterministic, multiscale numerical and empirical modeling approaches.

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MS43

Solving Differential Equations Numerically in the Chebfun System

Chebyshev spectral methods are a standard tool for solving numerical ODEs and PDEs to high accuracy. The chebfun system can be used to solve such problems with an adaptively determined polynomial degree. This technique has been abstracted using a new object class called chebops. These objects encapsulate matrices that can be realized at any size and incorporate boundary conditions automatically, so that the mechanics of spectral discretization are completely hidden from the casual user. Furthermore, standard MATLAB syntax, such as the backslash operator, has been overloaded to the context of linear operators on chebfuns. Using chebops one can solve a wide variety of initial-value, boundary-value, and eigenvalue problems in one space dimension numerically to high accuracy with a purely symbolic syntax.

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MS43

Polynomial and Rational Approximation in the Chebfun System

Theorems due to Ehlich and Zeller, Mastroianni and Szabados, Bernstein, Salzer, and Higham, explain the powerful approximation properties of chebfuns. But on the other hand, chebfuns can be used to explore and obtain new insights on computational aspects of approximation theory. In this talk we explain how to implement chebfun-based methods for some classical algorithms to construct different types of polynomial and rational approximates. In particular, we present a Remez algorithm based on chebfuns to compute best polynomial and rational approximations; near-best polynomial and rational approximations obtained with a Carathéodory-Fejér algorithm for chebfuns; and Padé and Chebyshev-Padé approximates implemented with chebfuns. Specific properties of these approximations are also discussed in the framework of chebfuns. All in all, we show that the chebfun approach to approximation theory is suitable for implementing various algorithms in a simple and efficient way while it also provides with a mechanism to explore many aspects of the theory on which they are based.

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MS43

Automatic Detection of Breakpoints for Piecewise Smooth Chebfuns

The original chebfun system, developed by Zachary Battles at Oxford during 2002-2004, dealt with smooth functions on $[-1, 1]$. We have now enhanced it in a major way by extending it to piecewise smooth functions on arbitrary intervals. Sometimes discontinuities are introduced implicitly via other operations, as in this example:

```
x = chebfun('x'); f = sin(10*x); h = max(f,x)
```

The result is a function with 8 smooth pieces manipulated to the usual machine precision. At other times discontinuities are introduced by a process of fast automatic edge detection, as in a case like this:

```
b = chebfun('abs(x-0.1)').
```

Now there are just two pieces, and machine precision as usual. The talk will outline the algorithms we have implemented and show how well they work (and how much fun they can be!) in practice.

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MS43

Introduction to Chebfuns and the Theorems They are Based On

The chebfun system is a class in object-oriented Matlab that computes with functions by using the same syntax that Matlab uses for vectors. Thus if f is the chebfun for bessel(x) on the interval [0,50], for example, we can compute its integral with sum(f), its maximum with max(f), or its roots with roots(f). All this is done to close to machine precision by methods based on Chebyshev expansions and interpolants: the system aims to"feel symbolic but run at the speed of numerics.' We begin the minisymposium with an online tour of the chebfuns in action.

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MS44

Delaunay Mesh Generation of Piecewise Smooth Surfaces, Volumes, and Complexes

Automatic mesh generation of various domains is an important goal in CAD. Recent sampling theory coupled with the Delaunay refinement strategy have proven to be effective for this problem. However, piecewise smooth surfaces and volumes remained as a challenge. Specifically, small angles subtended at non-smooth regions pose a serious obstacle to the strategy. In this talk we describe a method that removes the obstacle and can generate Delaunay meshes of piecewise smooth surfaces, volumes, and non-manifolds.

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MS44

Beyond Geometric Modeling in Aerospace

For several decades splines have been used as the primary mathematical technology in the construction of geometric models, both for engineering analysis and for manufacturing. With far less fanfare, splines have also been used extensively as a means of representing and communicating engineering data. This talk will explore some of the less celebrated, but nevertheless equally interesting, uses that splines have been put to at The Boeing Company, including mission planning, guidance and control, flight simulators, and electronic documentation.

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MS44

Geometry Processing in Industrial Design

The efficient processing of complex geometric models is a key requirement in most industrial design applications. As more stages of the workflow are mapped to digital models and numerical simulations, the generation, optimization, conversion, and storage of 3D models become important tasks in the overall process. In this talk I present algorithms that augment geometric raw data into consistent "watertight" polygon models which satisfy all the typical quality requirements for shape editing, simulation, and NC-manufacturing.

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MS44

Discrete Geometry for Virtual Worlds

Digitizing our 3D world with the same ease, speed and perfection as taking a digital picture photograph is becoming a key necessity in our daily life. Computer aided design, medical analysis, archeology, animation industry, fashion design, and e-commerce are just a few of the many industrial applications of digital 3D geometries. This talk introduces new ideas from discrete differential geometry having led to superior algorithms for geometry compression and surface remeshing, and their integration in industrial animation software.

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MS45

Bending with Local Geometrical Constraints

A variational framework is introduced to describe how a surface bends when it is subject to local constraints on its geometry. This framework is applied to describe the patterns observed in a folded sheet of paper. The unstretchability of paper implies a constraint on the surface metric; bending is penalized by an energy quadratic in mean curvature. The local Lagrange multipliers enforcing the constraint are identified with a conserved tangential stress that couples to the extrinsic curvature of the sheet. The framework is illustrated by examining the deformation of a flat sheet into a generalized cone.

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MS45

Curvature-Driven Lipid Sorting in a Membrane Tubule

Motivated by recent experiments that implicate the mechanical properties of membranes in lipid sorting, we examine the interplay of lipid composition and curvature in membrane tubules. We study how the coupling between membrane composition and membrane bending stiffness and tension affects tubule formation. Drawing a tubule from a vesicle leads to a rearrangement of composition in which the phase of higher flexibility segregates into the highly curved tubule. For point forcing, the force vs. extension curve can have a sharp drop just as the tubule begins to form.

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MS45
Non-Equilibrium Dynamics of Biomembranes

Lipid bilayer membranes that envelop cells and cellular organelles have unique mechanical properties crucial for biological function. Membranes constantly deform due to stresses naturally existing in the cellular environments or due to externally applied flow or electric fields. The past several years have marked an explosion in the interest in the genuine non-equilibrium states of membranes. However, progress in the theoretical analysis and numerical simulations has been slow because modeling membranes is a challenging task: membranes exhibit highly nonlinear behavior and involve multiple length scales. In this talk, I will discuss our recent advances in the theory of microhydrodynamics of closed lipid membranes (vesicles). I will present analytical results describing vesicle dynamics in uniform AC fields. The model quantitatively describes the experimentally observed behavior: as the frequency is increased, a vesicle filled with a fluid less conducting than the surrounding fluid undergoes a first shape transition from prolate to oblate ellipsoid, and then a second transition back to prolates.

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MS45
Molecular 'Hole Punchers' and Their Mechanisms: Relation Between Chemistry and Topology

Antimicrobial peptides comprise a key component of innate immunity for a wide range of multicellular organisms. It has been shown that natural antimicrobial peptides and their analogs can permeate bacterial membranes but not host membranes. There are a number of proposed models for this action, but the detailed molecular mechanism of the induced membrane permeation remains unclear. We systematically investigate interactions and self-assembled structures formed by model bacterial membranes and a prototypical family of phenylene ethynylene-based small molecule antimicrobials with controllable activity and selectivity. Synchrotron small angle x-ray scattering and confocal microscopy results correlate antibacterial activity and the induced formation of an inverted hexagonal phase, and indicate that the organization of negative curvature lipids such as DOPE are crucially important. Plate killing assays of DOPE-deficient mutant bacteria agree with the x-ray results. The general principles governing the action of membrane active antimicrobials are cognate to cell penetrating peptides such as TAT from the HIV virus and ANTP from the fruit fly. We will show that they both induce the negative Gaussian curvature topologically required for pore formation, and thereby generate a nanoporous double diamond bicontinuous cubic phase. Homologies as well as differences between these systems will be compared. Moreover, we will test our ideas using custom-designed cell penetrating block copolypeptides.

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MS46
Recent Advances in the What, How and When of Network Models in Infectious Disease Epidemiology

Not available at time of publication.

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MS46
Two Elementary Properties of Contagion Networks

The talk will introduce two new measures of centrality in the context of networked epidemiology: vulnerability and criticality. Informally vulnerability of an individual is the probability of the individual being infected. Criticality of a node refers to decrease in the vulnerability of other nodes in the network when the node is removed from the network. We show that interventions based on these new measures can be more effective than traditional measures such as node degree and betweenness in controlling epidemics. Highly efficient computational methods for computing these measures in very large social networks will also be discussed.

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MS46
Time Evolution of Disease Spread on Networks: Implications for Influenza Pandemic Preparedness

Currently, analytically tractable mathematical models of infectious diseases either address the time evolution of disease spread at the expense of simplifying the pattern of transmission, or incorporate detailed information pertaining to the contact structure among individuals while disregarding the time progression during outbreaks. We offer a new analytical framework, which incorporates both the complexity of contact networks and time progression of epidemics, and demonstrate how these tools can be utilized to refine pandemic preparedness guidelines.

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MS46
Title Not Available at Time of Publication

Not available at time of publication.

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MS47
Approximation of Partial Differential Equations with High-Dimensional Random Input Data

We first investigate the efficiency of some uncertainty propagation schemes for the solution of stochastic partial differential equations (SPDEs) with large number of input uncertain parameters. An efficient least-squares scheme is then introduced for a low-rank approximation of the solution of an SPDE with high-dimensional random input data. We will show that, in theory, the computational cost of the proposed algorithm grows linearly with respect to the dimension of the underlying probability space.

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MS47

The Use of Coarse-scale Models for Uncertainty Quantification of Porous Media Flows

In this talk, I will describe the use of coarse-scale models in uncertainty quantification. The problem under consideration is posed as a sampling problem from a posterior distribution. The main goal is to develop an efficient sampling technique within the framework of Markov chain Monte Carlo methods that uses coarsescale models and gradients of the target distribution. The purpose is to reduce the computational cost of Langevin algorithms for dynamic data integration problems. We propose to use inexpensive coarsescale solutions in calculating the proposals of Langevin algorithms. To guarantee the correct and efficient sampling of the proposed algorithm, we also intend to test the proposals with coarse-scale solutions. Comparing with the direct Langevin algorithm based on fine-scale solutions the proposed method generates a modified Markov chain by incorporating the coarse-scale information of the problem. Under some mild technical conditions we show that the modified Markov chain converges to the correct posterior distribution. Our numerical examples show that the proposed coarse-gradient Langevin algorithms are much faster than the direct Langevin algorithms but have similar acceptance rates.

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MS47

Stochastic Multiresolution Mathematical Analysis Framework–Integrated Materials Design to Molecular Bio-Regenerative Engineering

In the not too distant future, an integrated multiscale analysis system for the design of a reliable engineering structure to sustain harsh environmental conditions within a predetermined lifetime may be possible. In contrast to standard hierarchical homogenization analysis, the proposed multiresolution analysis framework will provide concurrent analysis of critical material, product structure, and manufacturing decisions in an integrated manner. Such capability is currently missing, but it is critical for achieving integrated material, product, and process design in a multiresolution, multiphysics design environment. The multiresolution mechanics theory is suitable for the analysis of the multiscale/multiphysics material systems such as fuel cells, self healing alloys, high strength alloys, high toughness alloys, microsystems, and thermoelectric materials. These nano/micro scale multi-functional materials are too large for first principles approaches, and too small for conventional FEA. The multiresolution mechanics connects all the scales dictated by the microstructure in a particular material. The key to developing advanced materials is the understanding of the interplay between the various physical scales present, from the atomic level interactions, to the microstructural composition and the macroscale behavior. New technological advances today allow for a range of advanced composite materials, including multilayer materials and nanofiber-matrix composites. By designing material microstructure intelligently, we may hope to create new materials with desired combinations of strength, toughness and density. The ability to do this will require new SBE&S methods that can be used to predict macroscale properties accurately based on microstructure (and nanostructure) without resorting to empiricism. A rigorous mathematical framework for multiscale modeling and material optimization will help to make super-lightweight, ultrastrength, low-wear materials a reality of everyday life—for energy related, industrial, and medical applications alike. In materials engineering, rather than randomly discovering materials and exploiting their properties, the goal is to develop a comprehensive understanding of microstructure-properties relationships in order to systematically design materials with specific desired properties.

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MS47

Efficient Implementation and Applications of Generalized Polynomial Chaos Methods

Generalized polynomial chaos (gPC) has become one of the most widely used methodology for uncertainty quantification and stochastic simulations. In this talk we discuss efficient implementations for some stochastic systems, including effective decoupling of the gPC Galerkin system for random diffusions. We will also discuss applications of gPC to Bayesian analysis and data assimilation.

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MS48

FETK and Applications to Geometric PDE

In this lecture, we give an overview of the Finite Element ToolKit (FETK), which is a collaboratively developed set of open source finite element modeling software libraries for nonlinear elliptic and parabolic partial differential equations (PDE) on general 2D and 3D spatial domains. The FETK software has been designed primarily to solve coupled nonlinear elliptic and parabolic geometric PDE on domains having the structure of Riemannian manifolds, but is also efficient for more standard problems on open sets on R2 and R3. At the core of FETK is an adaptive finite element method (AFEM), which has been developed in accordance with modern AFEM convergence theory. As a result, the adaptive algorithm in FETK can be shown to be a strict contraction in the sum of the error and error-indicator measures, and in addition can be shown to have optimal complexity for a broad range of nonlinear problems including those with non-monotone nonlinearities. We show some examples of the application of FETK to two challenging 3D nonlinear elliptic problems: the Poisson-Boltzmann equation arising in biophysics, and the Einstein constraint equations arising in gravitational wave models.

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MS48

A Fully-Automatic HP-Adaptive Finite Element Method for Maxwell's Equations in 3D

We describe our algorithm for fully-automatic hp-adaptive mesh refinement in three dimensions. The generated (hexahedral) meshes allow full anisotropy in both element size h and order of approximation p, and are shown to deliver exponential convergence of the error (in either a global energy norm or a given quantity of interest) with respect to the problem size, even in the presence of singularities. The method is applied to the analysis of several 3D electromagnetic waveguides.

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MS48

OOF: An Object-Oriented Finite Element Solver for Materials Science

PDEs arise naturally in many scientific fields in which the investigators are not themselves PDE experts. These researchers can benefit from PDE software that speaks the language of their field, and presents the mathematics in a straightforward way. The OOF finite element software, intended for a materials-science audience, aims to provide push-button access to advanced mesh construction and equation solving tools, simplifying PDE solving for real-world materials problems with complex geometries.

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MS48

Toward Adaptive Finite Element Simulations on Petascale Computers

Parallel adaptive finite element simulations requires the ability to control the evolving workload and communications of changing meshes. We have previously developed parallel adaptive procedures that have been applied on clusters of up to a few hundred processors. This talk will discuss recent developments of parallel adaptive finite element methods for massively parallel computers approaching 100,000, or more, processors and present our latest results on a 32,000 processor IBM Blue Gene.

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MS49

Multilinear Algebra Based Fitting of a Sum of Exponentials to Oversampled Data

We present a high-precision method for the estimation of the parameters of a signal, modelled as a finite sum of complex damped exponentials, whose poles may be close. The solution follows from the computation of the dominant subspace of the column space of a third-order tensor.

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MS49

Large-Scale Tensor Computations and Applications to Data Mining

A tensor is a multidimensional or N-way array. Tensor decompositions have recently become popular in a wide variety of fields, including biology, medicine, chemistry, computer science, and engineering. Computational tools, however, are still somewhat rare and the challenge of handling large-scale data is just beginning to be addressed. In this talk, we survey the state-of-the-art in large-scale tensor computations. Many of the large-scale problems arise in data mining applications, so we also present motivating problems in this domain.

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MS49

A Novel Higher-Order Generalized Singular Value Decomposition for Comparative Analysis of DNA Microarray Data From Different Organisms

We define a higher-order generalized singular value decomposition (GSVD) of more than two matrices D_i of the same number of columns and, in general, different numbers of rows. Each matrix is factored as $D_i = U_i \Sigma_i V^T$, where the columns of U_i and V have unit length and Σ_i is diagonal. We show that this decomposition extends to higher-orders most mathematical properties of the GSVD and enables comparison of large-scale datasets, such as DNA microarray data from different organisms.

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MS49

Multilinear Algebra Computations in Quantum Chemistry

The simulation of complex quantum chemical systems of interacting electrons leads to a number of high dimensional tensor computations. In this talk we will highlight the advantages of low-rank approximation and block tensor data structures.

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MS50

Generalized Maxwell Model for Inelastic Polar Rods. Application to Self-Organization of Microtubules and Molecular Motors

We derive a model describing spatiotemporal organization of an array of microtubules interacting via molecular motors. Starting from a stochastic model of inelastic polar rods with a generic anisotropic interaction kernel, we obtain a set of equations for the local rods concentration and orientation. At large enough mean density of rods and concentration of motors, the model describes an orientational instability resulting in spontaneous ordering. We study the existence and dynamic interaction of microtubule bundles analytically and numerically. Our results show a long term attraction and coalescing of bundles indicating a clear coarsening in the system.

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MS50

Kinetic Models for Wave Propagation in Media with Random Scatterers

Waves propagating in random media with discrete scatterers undergo significant scattering when the so-called mean free path is comparable to or smaller than the overall distance of propagation. In certain situations, the wave energy density may be modeled by a radiative transfer equation and, moreover, the wave energy density becomes statistically stable, i.e., independent of the realization of the random medium. In such cases, the radiative transfer equation may be used as an accurate forward model to image an unknown medium. We apply the method to the imaging of inclusions buried in random media.

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MS50

Phase Transition with Non-Thermodynamic States in Reversible Polymerization

We investigate a reversible polymerization process in which individual polymers aggregate and fragment at a rate proportional to their molecular weight. We find a nonequilibrium phase transition despite the fact that the dynamics are perfectly reversible. When the strength of the fragmentation process exceeds a critical threshold, the system reaches a thermodynamic steady state where the total number of polymers is proportional to the system size. The polymer length distribution has a sharp exponential tail in this case. When the strength of the fragmentation process falls below the critical threshold, the steady state becomes non-thermodynamic as the total number of polymers grows sub-linearly with the system size. Moreover, the length distribution has an algebraic tail and the characteristic exponent varies continuously with the fragmentation rate.

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MS50

Scaling Dynamics in Min-Driven Coagulation Models

We study mean-field models of the evolution of domain size distributions, motivated by the phemenon of domain coarsening in the one-dimensional Allen-Cahn PDE. We extend a remarkable solution procedure for these models, found by Gallay and Mielke, to establish: dynamical well-posedness in the space of probability measures; a well-posedness theorem for measure-valued size distributions; necessary and sufficient conditions for approach to self-similar form; and a Levy-Khintchine representation formula for eternal solutions.

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MS50

On New Stochastic Kinetic Models of Non-Ideal

Fluids

We consider a new liquid-state kinetic theory for particles with interaction potentials that are continuously varying (such as Lennard-Jones particles and inverse-power-law potentials), rather than discontinuous (such as the hard-sphere or square-well potentials). We do this by incorporating a stochastic smoothing term at the hard-core and the square-well edge of the square-well kinetic model (KVTIII). The resulting kinetic model has built in conservation laws and trend to equilibrium (H-functional). We derive and evaluate the virial coefficients and transport coefficients for the underlying fluid. We also consider existence and stability results for the corresponding system of the kinetic equations.

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MS51
Mimetic Discretization of Sediment Transport Equations

In this study, we using mimetic methods to develop a numerical model for the simulation of the load sediment transport under the water velocity condition giving by shallow water equations. This model consist of two modules, first by a bi-dimensional circulation model, and a second for a load sediment transport model. Both modules are resolved with mimetic techniques, which they have shown to be very efficient due to that this type of schemes take account laws of conservation of the physical problem. The model is tested with simple geometries for its validation, being behaved adequate.

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MS51
Evaluating the Relative Importance of the Terms of the Navier-Stokes

The relative importance of each term of the movement equations was evaluated using information from HF radars for the Pacific U.S.-Mexico border region. A set of equations that describes the vertically averaged horizontal velocities was obtained using the continuity and movement equations. This set of continuous equations was made discrete using finite differences and the trapezoid method for integration. The equations, in their discrete form, were evaluated using a time series of superficial velocities for the Pacific U.S.-Mexico border region, measured by a system of HF radars in 2003. A computational algorithm that calculates the relative contribution of each term of the equations was applied. The HF radar system, combined with the proposed method, proved to be useful to study the contribution of each term to the movement equations for superficial currents covering extensive regions and to classify the zones of the study area by means of dominate physical budgets using eulerian measurements. The analysis performed demonstrates that, in the study region, onshore is influenced by the geostrophic budget (47%), while offshore was affected by the inertial budget (46%).

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MS51
Monitoring of Particulate Organic Carbon Using Satellite Ocean Color Observations

Algorithms linking optical properties to chlorophyll concentration in the ocean have been the focus of numerous studies. However, for ocean biogeochemistry and climate studies it is carbon, not chlorophyll, which is of most direct interest. I will present our work on estimating the ocean surface particulate organic carbon (POC) concentration using optical satellite measurements. I will also discuss our future plans to use satellite derived POC maps to study oceanic POC budgets and fluxes.

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MS51
Full 3-D General Curvilinear Modeling of the Monterey Bay

Monterey Bay (MB) is the largest bay of the West Coast of the United States. It is characterized by a complex coastline and regions of steep bathymetry. Local upwelling events and strong land/sea breeze influence circulation patterns in this area. Topographical characteristics as well as atmospheric and oceanographic conditions and processes make the MB region ideal to exploit the capabilities of a 3D curvilinear ocean model such as the General Curvilinear Ocean Model, GCOM. GCOM is based on the non-hydrostatic, non-linear primitive equations for momentum and density in the f-plane. It is capable to handle the complex combination of rotation and abrupt bathymetry. It has been used succesfully to model flow circulation and density evolution in a variety of places with different coastline and shape basins such as The Gulf of Mexico, The Gulf of California, The Bahia de Todos Santos in Mxico. For the Monterey Bay case, density and velocity fields are presented for various flow conditions.

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MS52
Enriched Multi-Point Flux Approximation for General Grids

The two-point flux approximation, a numerical scheme used in most commercial reservoir simulators, has O(1) error when grids are not K-orthogonal. The multi-point flux approximations have been developed as a remedy. However, non-physical oscillations can appear when the anisotropy is really strong. We present the recently developed control volume enriched multi-point flux approximation (EMPFA) for general diffusion problems on polygonal and polyhedral meshes. Non-physical oscillations are not observed for realistic and strongly anisotropic heterogeneous material properties described by a full tensor. Exact linear solutions are recovered for grids with non-planar interfaces, and a first and second order convergence are achieved for the flux and scalar unknowns respectively.

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MS52

Discontinuous Galerkin Solver for Boltzmann-Poisson Equations

We present results of a discontinuous Galerkin scheme applied to deterministic computations of the transients for the Boltzmann-Poisson system describing electron transport in semiconductor devices. The collisional term models optical-phonon interactions which become dominant under strong energetic conditions corresponding to nano-scale active regions under applied bias. The proposed numerical technique is a finite element method using discontinuous piecewise polynomials as basis functions on unstructured meshes. Both one-dimensional and two-dimensional examples will be given, demonstrating the advantages of this scheme compared to other deterministic solvers. This method also has great promise for adaptivity, which will be addressed in the future.

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MS52

Multigrid Solvers for Symmetric Interior Penalty Methods on Graded Meshes

In this talk we discuss multigrid solvers for systems resulting from the discretization of second order elliptic boundary value problems by symmetric interior penalty methods on graded meshes. We will present both theoretical and numerical results. This is joint work with Susanne C. Brenner and Li-yeng Sung.

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MS52

Transport Simulations with Spectral Element Discontinuous Galerkin Methods

I will present progress in developing SEDG-based methods for solving electromagnetic wave propagations and lattice Boltzmann flow problems. I will discuss our high-order solver, NekCEM, for large scale simulations on wake potential calculations for complex geometries on accelerator components. Accuracy and performance compared to conventional low-order methods will be demonstrated. As an alternative method for solving flow problems based on the Navier-Stokes equations, we developed spectral element lattice Boltzmann (SELB) method with discontinuous Galerkin approach. We will demonstrate some prototype sigle-phase flow simulations obtained by the SELB method. This is joint work with P.F. Fischer (Argonne National Laboratory), T. Lee (The City University of New York), and Yong-Chul Chae (Argonne National Laboratory).

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MS53

Conformal Mapping of Multiply Connected Domains: An Overview of Some Recent Methods

A brief overview of two classes of methods developed in recent years for computing conformal maps of multiply connected domains will be given. The first class of methods extends the Schwarz-Christoffel formula for mapping circle domains to domains with polygonal boundaries and can be formulated using reflection arguments or Schottky-Klein prime functions. The second class of methods maps from circle domains to domains with smooth boundaries and is based on Fourier/Laurent series or Riemann-Hilbert problems (due to R. Wegmann). Progress on the numerical implementation of these methods and their relation to other talks in this minisymposium will be given.

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MS53

Least Squares Methods for Conformal Mapping and Boundary Value Problems

Many conformal maps and related boundary value problems in potential theory are analytic or harmonic at all but a few points, with singularities whose structure is known in advance. Accordingly, they can be expressed as linear combinations of smooth and singular terms. When one can formulate linear conditions for the solution to satisfy on the boundary, discretization leads to standard linear least-squares problems that can be solved quickly. If one takes care to avoid ill-conditioned bases, for example by using the Arnoldi iteration, then one can realize, with short, simple computer programs, methods that give fast and accurate solutions to problems with piecewise smooth boundaries and simple or higher connectivity.

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MS53

Radial and Circular Slit Maps of Multiply Connected Domains

Infinite product formulas for conformally mapping a multiply connected circle domain to a canonical radial or circular slit domain are derived. The formulas are generated by analytic continuation with the reflection principle. Convergence of the infinite product is proved for domains with sufficiently well separated boundary components. Some recent progress in the implementation and application of the formulas is presented. This is joint work with T. DeLillo, T. Driscoll, and J. Pfaltzgraff.

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MS53

Riemann-Hilbert Problem for Multiply Connected Domains

We solve the scalar Riemann-Hilbert problem for circular multiply connected domains. The method is based on the reduction of the boundary value problem to a system of functional equations (without integral terms). In the previous works, the Riemann-Hilbert problem and its partial cases such as the Dirichlet problem were solved under geometrical restrictions to the domains. In the present work, the solution is constructed for any circular multiply connected domain in the form of modified Poincare series.

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MS54

High-Speed Flow Solvers for Overlapping Grids

In this talk we discuss the implementation of high Mach number compressible flow solvers in the context of overlapping grids. The overlapping mesh infrastructure is discussed, including general characterization of structured overlapping meshes, adaptive mesh refinement, and relative mesh motion. Two classic high speed flow solvers, a high resolution Godunov type method and flux-corrected transport, are presented, suitably modified for overlapping meshes, and a series of test problems are presented to showcase the relative virtues of each scheme. Finally a set of more complicated problems is introduced and the results obtained using each scheme are compared.

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MS54

Studies of Compressible Flows Using Arbitrary-order Hermite Discretizations

Hermite methods allow the construction of stable, high-order discretizations of pdes on structured grids. They are characterized by the use of local polynomial expansions rather than simple point values as nodal data. We describe our Hermite-based compressible flow solver and demonstrate its performance through the simulation of various complex flows. We also discuss the imposition of boundary conditions and test simple strategies for p-adaptivity and shock capturing.

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MS54

A Hybrid Method for the Unsteady Compressible Navier-Stokes Equations

A hybrid method composed of finite difference-finite difference and finite difference-finite volume schemes for the time-dependent Navier-Stokes equations has been developed. A detailed analysis of the stability of the proposed algorithms, paying special attention to the stability of the interfaces between the subdomains is performed. We prove that the interface coupling is stable and conservative. The efficiency and applicability of the procedure is exemplified by considering a range of compressible flow problems including complex geometries and shocks.

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MS54

New Concepts for Developing Nonoscillatory Methods for Hyperbolic Conservation Laws

The development of various non-oscillatory methods has been linked to the concepts of monotonicity and total variation through nonlinear stencil selection. Extending these methods to higher formal order of accuracy such as ENO methods has preceded using concepts only tenuously connected. Here, the total variation diminishing methods are extended conceptually to produce ENO methods with improved accuracy and stability. The new methods have properties more amenable to analysis providing a greater level of formality.

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MS55

Numerical Simulation and Application Studies of Multiscale Coupled Physics Problems using Libmesh

We have been developing methods, algorithms and an open-source software library Libmesh for parallel adaptive multiphysics simulation. Here we describe some aspects of our recent research and application studies for coupled flow and heat transfer , biomedical applications, interfacial problems, coupled porous media flows and complex variable coupling. The material will also include some recent work coupling libmesh with monte carlo statistical software library DAKOTA. Numerical performance studies for this class are also included.

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MS55

Applying Newton-Krylov Methods to Multiphysics/multicode Systems and a Path to Quantifying Coupling Strength

We have applied Newton-Krylov techniques to pre-existing production simulation tools to achieve near-Newton convergence rates. This was done in a non-invasive way to minimize the effort required to couple different simulation methods together. In addition, we have begun investigating issues related to how well the off-diagonal blocks in the preconditioner must be approximated to attain reasonable convergence rates.

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MS55

Issues in Software for Coupled Multiphysics PDEs

Employing numerical software libraries in the context of coupled multiphysics PDE-based models raises numerous challenges. As motivated by coupling in fusion and accelerator simulations, we are developing capabilities to facilitate the construction of multimodel algebraic solvers. This talk will introduce an approach for multimodel algebraic system specification, with emphasis on providing the flexibility for application programmers to specify subsets of physics from which subsolvers may be efficiently constructed.

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MS55

Iterative Techniques for the Solution of Coupled Multiphysics Problems

We investigate the iterative solution of multi-physics problems using a multi-discretization operator decomposition approach. We demonstrate that the standard iterative coupling schemes correspond to block Jacobi and block Gauss-Seidel algorithms and frequently diverge. We derive an alternative technique based on an inner Newton-Krylov iteration and the solution of a variational system, and show that this approach is a generalization of a preconditioning technique used in domain decomposition. We provide numerical results to show that this Newton-Krylov approach can significantly reduce the overall cost in computing iterative solutions to coupled multi-physics problems.

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MS56

Modeling Neural Subcircuits in the Outer-Plexiform Layer of the Retina

Image processing in the retina begins in the outer plexiform layer, where bipolar, horizontal, and photoreceptor cells interact. We mathematically model the subcircuits of the outer plexiform layer and investigate if feedback effects in the cone photoreceptor's synapse are driven by electrical (ephaptic) or chemical (neurotransmitters, e.g., GABA) mechanisms.

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MS56

Numerical Methods for Electro-Reaction-Diffusion Modeling of Biological Cells

Electro-reaction-diffusion models and numerical methods for their solution will be discussed for simulating various properties of biological cells involving ion transport, including ion propagation through channels in the cell membrane and electrical signals in nerve cells. Robust numerical methods (especially TRBDF2 for the time integration) needed to solve these stiff nonlinear differential equation models – which include advection-diffusion and reaction-diffusion PDEs, Poisson's equation, and ODEs for modeling ensembles of channels – will be emphasized.

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MS56

Numerical Methods for a Model of Calcium Waves in a Human Heart Cell

The flow of calcium ions in a heart cell is modeled by a system of transient reaction-diffusion equations. The large number of point sources to model the injection of calcium ions and the requirement for high-resolution meshes are among the challenges for convergent and efficient numerical methods for this problem. I will describe the techniques used for long-time simulations of this model on a distributed-memory cluster, while ensuring the accuracy of several crucial physical properties of the solution.

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MS56

Waves of Cortical Spreading Depression

Waves of cortical spreading depression (CSD) in various brain structures are characterized by depression of the EEG and massive changes in ionic concentrations. In humans, migraine with aura is associated with CSD waves in the visual cortex. CSD waves are accompanied by reduced electrical activity in neurons. We review CSD wave propagation properties and describe some physiological mechanisms that appear to be important for CSD waves. Nonlinear diffusion equation models for CSD will be described.

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MS57

Recommendations for Change: Why and How National Policies for Change: A Brief Survey

This two-part talk will first describe the BIRS report, then give a quick tour of related national policies. The recommendations in the BIRS report are addressed to individuals, administrators, and policymakers in the mathematical sciences. They encourage action by mathematics institutes, funding bodies, university administrations, mathematics departments, and department chairs. Related national policies are in place or have been proposed. The US Gender Bias Elimination Act is an example of the latter.

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MS57

Building Gender Equity in Mathematics: The Nebraska Experience

I will discuss efforts that are being undertaken at the University of Nebraska to build gender equity in mathematics. These include programs designed to encourage women to enter careers in mathematics as well as efforts to create a climate in which all qualified people can be successful.

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MS57

Gender Equity Workshops for Chairs of the Top Physics and Chemistry Departments in the U.S.: Whats the Impact?

Two federally funded workshops for physics and chemistry department chairs were held recently with the common goals: to educate chairs on the issues surrounding gender equity, and to help them to develop and implement plans to increase gender diversity in their departments. This presentation summarizes the results of research conducted by COACh on the short and long-term impact of these workshops on participating departments and presents insights into the ingredients necessary to make such at effort successful.

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MS57

Retaining Women in the Field of Mathematics, The Importance of Mentoring and How MentorNet Can Make a Difference

Recruitment of women and under-represented populations into the field of mathematics has received substantial attention. Recruitment isnt enough; retention activities are important in the undergraduate and graduate programs. Mentoring is one strategy that has proven successful in helping retain women in their undergraduate and graduate programs. MentorNet has ten years of experience, and national recognition of its benefit, in helping retain women and under-represented populations. Successful mentoring is more than just connecting two people together.

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MS58

Curvature Estimation Methods for Simulation of Multi-Material Flows with Interface Tracking

Estimation of interface curvature is important for simulating flows with surface tension such as bubble formation and growth, dendritic growth etc. In this talk we propose a new method for estimating curvature in the (Volume-of-Fluid) VOF method and compare it existing methods. We ¿also propose a new method for estimating interface curvature in the ¿Moment-of-Fluid (MoF) method.

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MS58

Non Conformal Adaptation and Smoothing Mesh

for Compressible Lagrangian Fluid Dynamics

For the numerical approximation of two-dimensional compressible Lagrangian fluids dynamics, we propose a three steps strategy. We begin with a centered Lagrangian scheme, then we perform an adaptation step based on a variant of local non conformal cells. Here the new added nodes can be degrees of freedom exactly as the master nodes, so that we call them semi-slaves. Finally, we do a rezoning with nodal mesh quality control followed by a remapping.

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MS58

Evaluating Volume Fractions in Arbitrary Hexahedral ALE-AMR Zones for Non-onion Skin Multi-Material Interface Reconstruction

We present a method applicable to multimaterial interface reconstruction for exactly evaluating the partial volumes of arbitrary hexahedral zones truncated by multiple planar interfaces. The key advantages of this method are that approximate geometric decompositions are avoided and that the truncating interfaces may intersect one another within the zone, whereas previous exact methods have been limited to onion skin topologies. We demonstrate the method in geometry definition and adaptive mesh refinement in ALE-AMR.

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MS58

Multimaterial Multiphysics in ALEGRA

ALEGRA is a multiphysics code developed at Sandia National Laboratory. ALEGRA is used to simulate a broad spectrum of physical problems ranging from the magnetically driven implosions to shock loaded evolution of exotic materials. Each of these problem areas has diverse requirements for successful simulation. In particular the code implements MHD, advanced solid mechanics and radiation transport in conjunction with the evolution of multiple materials. This presents distinct challenges for development of accurate robust algorithms.

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MS59

Orthogonal Representations of Generalized Stochastic Processes

In recent years, orthogonal representations of random variables and processes using the Karhunen-Loeve expansion and the Polynomial Chaos expansions have been used in conjunction of various constrained such as partial differential equations to characterize the probabilistic structure of stochastic processes with particular mathematical structures. In this presentation, we present a general description of stochastic processes that naturally permits the integration of a variety of such constraints. This is done by construing the stochastic processes of interest as members of a suitably constructed functional space. Specifically, we extend the Karhunen-Loeve expansion to vectorvalued stochastic processes with particular attention to distribution-valued processes. In the process, we explore the structure of the associated reproducing kernel Hilbert spaces (RKHS) and the weak form of the associated eigenvalue problem. We identify the role that the dual of the phase space of the stochastic process plays in the analysis of this problem. We show the significance of our presentations to various model reduction formalisms.

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MS59

Optimization of Radio-Frequency Ablation in the Presence of Material Parameter Uncertainty

We present an approach for the optimization of the probe placement in radio-frequency (RF) ablation which takes the uncertainty associated with tissue properties (electrical and thermal conductivity) into account. Since in-vivo tissue properties are mostly unknown, have significant error margins, and are individually different, we consider them as having certain (probabilistic) distributions of values. Our forward simulation of RF ablation is based upon a system of partial differential equations (PDE) that describe the electric potential of the probe and the steady state of the induced heat. The probe placement is optimized by minimizing a temperature-based objective function such that the volume of destroyed tumor tissue is maximized. We discuss the sensitivity of the optimal probe placement under variations of the material parameters and we investigate the probe placement for which we expect maximal volume of destroyed tumor tissue. This leads to an optimization problem with a constraining system of stochastic PDE. This talks describes the derivation of the Euler-Lagrange equations as the necessary condition for the optimal probe placement. This system is solved with a multi-level gradient descent approach using a stochastic collocation method and finite elements on three-dimensional hexahedral grids. We underscore the usefulness of the approach by applying the optimization to scenarios from real RF ablations.

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MS59

Quantification of Chaotic Mixing Through Direct Numerical Simulation of Acceleration Driven Fluid Instabilities

Front tracking simulations of Rayleigh-Taylor and Richtmyer-Meshkov instabilities have revealed chaotic structure of the fluid interface. The solutions are lack of point-wise convergence. To quantify the mixing, we apply several strategies to the direct numerical simulation. This includes isolation of primary waves and flow regions with comparable history, analyze statistical properties, and quantify the ensemble average. Another method to quantify the turbulent mixing is through Fourier spectral analysis with comparison to the Komogorov theory.

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MS59

Nonparametric Bayesian Density Estimation via Polynomial Chaos Expansions

Characterizing random quantities from limited noisy observations is a problem in density estimation. We formulate a hierarchical Bayesian method for estimating polynomial chaos representations of such quantities, evaluating likelihoods with a Sturm-sequence polynomial solver. We introduce a reversible-jump Markov chain Monte Carlo scheme that simultaneously explores the polynomial degree and corresponding coefficients, thus allowing an infinitely parametric representation of the underlying random variable. Results include examples in systems reliability, with extensions to multivariate problems.

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MS60

Teaching Numerical and Symbolic Computation using Open Source Software

Open source alternatives are now available in python that can provide nearly all of the functionality required for teaching most applied mathematics courses. Python has the additional advantage of being far more powerful and generally useful than any single commercial package. The SAGE software provides a common interface to both numerical and symbolic software and also provides a simple interface to Fortran, C, LaTex, and other languages. I will present some examples of how this might be used in teaching applied mathematics courses.

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MS60

NumPy and SciPy: Open Source Tools for Numerical Computing in Python

NumPy and SciPy form the foundation of numerical computing in Python. NumPy provides sophisticated multidimensional arrays, with similarities (but more flexible capabilities) to Fortran90 or Matlab arrays, as well as linear algebra libraries, FFTs and facilities for interfacing with Fortran codes. SciPy provides additional libraries for scientific computing in areas such as signal and image processing, optimization, integration, and sparse linear algebra. SciPy is actively developed by a growing community of scientists from multiple disciplines.

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MS60

Python: A Scalable Tool for Scientific and Mathematical Computing

Python is an open source, high level language that is rapidly growing as an alternative to proprietary systems for scientific computing. It can be used from interactive numerical exploration and prototyping to large scale application development, including low-level Fortran and C/C++ libraries, symbolic manipulation, data visualization, distributed computing and graphical interfaces. This talk will be a high-level overview of its uses and capabilities; specific projects will be discussed in detail throughout the minisymposium.

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MS60

Sage: A Unified Environment for Mathematical Computation

I will describe SAGE, which is software for studying a huge range of mathematics, including algebra, calculus, statistics, number theory, cryptography, numerical computation, commutative algebra, group theory, combinatorics, graph theory, and exact linear algebra. SAGE is based on the Python language and can be used from a web browser, which connects either to a local or remote SAGE kernel. With the SAGE notebook you can create embedded graphics, beautifully typeset mathematical expressions, and more.

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MS61

Pseudo-Transient Continuation

Pseudo-transient continuation (PTC) computes steady state solutions of time-dependent problems by integrating the dynamics to steady state using very large time steps. In this talk we will give an overview of the method, show how it can be adapted to constrained nonlinear equations, and discuss some new applications.

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MS61

Applications of Jacobian-free Newton Krylov Technique

We present recent progress in applications of Newtons method to applied problems modeled by partial differential equations: from penalized spline continuum representation of particle densities, mesh control, and multiphysics coupling in the modeling of fusion plasmas, to distributed parameter identification in the Fitzhugh-Nagumo system of reaction-diffusion equations. These diverse topics share a common mathematical structure and parallel software interface in the Jacobian-free Newton-Krylov method.

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MS61

Physics-based Preconditioning of Jacobian-Free Newton-Krylov Methods

The Jacobian-Free Newton-Krylov (JFNK) method is increasingly being applied as the nonlinear solver for implicitly discretized multiphysics problems. The key to the efficient implementation is effective preconditioning. Legacy operator split and semi-implicit algorithms frequently exist for problems of interest. These algorithms are typically first-order accurate in time and contain uncharacterized stability constraints. On the positive side, these legacy algorithms have been developed with good physical insight and are CPU efficient per time step. A number of such solvers have been effectively applied as preconditioners for the JFNK method. We provide some details behind this concept along with some recent results from solidifying flow, magnetohydrodynamics, and low-speed viscous compressible flow.

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MS61

Inexact Newton Methods for Large-Scale Underdetermined Systems

Underdetermined nonlinear systems, i.e., nonlinear systems with more unknowns than equations, occur in a variety of applications. In the large-scale case, when iterative linear algebra methods are preferred, an inexact-Newton solution algorithm is appropriate. We formulate general inexact-Newton algorithms suitable for this context, outline local and global convergence results, discuss Newton-

Krylov implementations, and report on numerical experiments with a Newton-GMRES implementation applied to solving parameter-dependent systems and to determining periodic solutions of time-dependent problems.

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MS62
Social Query Models

Decentralized search by routing queries over a network is fast emerging as an important research problem, with potential applications in different areas, e.g., social networks, sensor networks, peer-to-peer networks. This talk will introduce a novel Social Query Model (SQM) for decentralized search, which factors in realistic elements such as expertise levels and response rates of nodes, and has the Pagerank model and certain Markov Decision Processes as special cases. We will present an efficient distributed algorithm for computing the near-optimal query routing policy in the SQM. Extensive experiments on both simulated random graphs and real small-world networks demonstrate the potential of the SQM model and the effectiveness of the proposed routing algorithm.

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MS62
Partitioning Large Graphs and Community Structure in Large Social Networks

Identifying communities in networks is one of the fundamental interests of network analysis, where communities are usually thought of as sets of nodes that interact more strongly with each other than with the remainder of the network. In this work we investigate some statistical properties of such communities in large real-world networks. In particular we investigate how a well known measure of community quality, the conductance score, varies with the size of the community. We study this question for almost 100 large real-world networks, and observe a counterintuitive inverse relationship between the optimal quality and size, which is exactly the opposite of what we would expect based on experience with both large spatial graphs and small social networks. We then discuss the underlying intuitions and the algorithmic and modeling implications of this observation.

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MS62
Classification in Sparsely Labeled Networks

We will address the problem of classification in a partially labeled network (a.k.a. within-network classification), with an emphasis on tasks in which we have very few labeled instances to start with. Recent work has demonstrated the utility of collective classification (i.e., simultaneous inferences over class labels of related instances) in this general problem setting. However, the performance of collective classification algorithms can be adversely affected by the sparseness of labels in real-world networks. We will show that on several real-world data sets, collective classification appears to offer little advantage in general and hurts performance in the worst cases. We will motivate a complimentary approach to within-network classification that takes advantage of network structure. Our approach is motivated by the observation that real-world networks often provide a great deal more structural information than attribute information (e.g., class labels).

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MS62
Social Networks in Collaborative Rating of Information

The rise of social media sites, such as blogs, wikis, Digg and Flickr among others, underscores a transformation of the Web to a participatory medium in which users are actively creating, evaluating and distributing information. The social news aggregator Digg allows users to submit links to and vote on news stories. Like other social media sites, Digg also allows users to designate others as "friends" and easily track friends' activities: what new stories they submitted, commented on or liked. Each day Digg selects a handful of stories to feature on its front page. Rather than rely on the opinion of a few editors, Digg aggregates opinions of thousands of its users to decide which stories to promote to the front page. We study how collaborative rating and promotion of news stories emerges from the independent decisions made by many users. We construct a mathematical model that takes into account user behavior: e.g., whether they read stories on the front page or get story recommendation through their social networks. Solutions of the model qualitatively reproduce the observed dynamics of votes received by actual stories on Digg.

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MS63
Discontinuous Galerkin Methods for the Chemotaxis Model and Closely Related Biomedical Problems

In this work, first, we propose a family of interior penalty discontinuous Galerkin methods for the Keller-Segel chemotaxis model. This model is described by a system of two nonlinear PDEs: a convection-diffusion equation for the cell density coupled with a reaction-diffusion equation for the chemoattractant concentration. It has been recently shown that the convective part of this system is of a mixed hyperbolic-elliptic type, which may cause severe instabilities when the studied system is solved by straightforward numerical methods. Therefore, the first step in the derivation of the proposed methods is made by introducing the new variable for the gradient of the chemoattractant concentration and by reformulating the original Keller-Segel model in the form of a convection-diffusion-reaction system with a hyperbolic convective part. We then design interior penalty discontinuous Galerkin methods for the rewritten Keller-Segel system. Our methods employ the central-upwind numerical fluxes, originally developed in the context of finite-volume methods for hyperbolic systems of conservation laws. We prove error estimates for the proposed high-order discontinuous Galerkin methods. Our proof is valid for pre-blow-up times since we assume boundedness of the exact solution. We also show that the blow-up time of the exact solution is bounded from above by the blow-up time of our numerical solution. In the numerical tests that will be presented, we first compare three different discontinuous Galerkin schemes applied to the Keller-Segel model: 1) primal discontinuous Galerkin methods applied to the original formulation of the Keller-Segel model, 2) primal discontinuous Galerkin methods with the standard upwind numerical fluxes for the reformulated Keller-Segel model and, 3) the new discontinuous Galerkin methods. We show, that compare to the new discontinuous Galerkin methods, the first two schemes fail to give the accurate, oscillation free solutions for the classical Keller-Segel chemotaxis model. Second, we will discuss some applications of the proposed discontinuous Galerkin scheme, to biomedical problems.

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MS63

Mesh Control for Large-Scale High Order Finite Element Simulations

High-order finite element method characterized by its higher rates of convergence can provide an effective means to address critical simulation-based applications with dramatically reduced levels of computational effort. However, when applying higher order finite element to complex 3-D domains, difficulties that arise are the need to have optimal meshes to account for the curved boundaries and thin sections. This talk is to present several mesh control techniques to construct curvilinear meshes for the usage of large-scale SciDAC applications. Higher order finite element method need curved meshes for complex curved 3-D domains. The common approach to the construction of such meshes is to take advantage of available mesh generators to apply straight-sided mesh generation and then curve the mesh edges and faces to curved domain boundaries. However, the resulting meshes often contain invalid because curving the mesh entities to model boundaries can lead to negative determinant of Jacobian in the closures of some elements. A procedure has been developed to apply curved local mesh modification operations to incrementally correct the invalid elements created during the mesh curving process. The curved local mesh modifications are applied in an order that effectively make the resulting curved elements valid[1]. This procedure ha been successfully applied to meshes used by Standford Linear Accelerator (SLAC) in the large-scale electromagnetic modeling of accelerator systems. The valid curvilinear meshes not only make the time-domain simulations stable but also improve the computer execution time up to 30 percent due to better conditioned matrices. The generation of curved meshes to support multiphysics simulations introduces an additional difficulty when the 3-D geometries contain complex thin structural walls, where multiple curved elements through thin section are needed. A procedure under development is to use a set of discrete computed medial surface points to automatically isolated the thin sections for the complex geometry and construct curved anisotropic layered elements through the thickness with properly order. The procedure can generate curved meshes with substantial less elements to save computational cost for large-scale simulations.

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MS63

Spectral Deferred Correction Methods with High Order Runge-Kutta Schemes

Spectral deferred correction (SDC) methods for ordinary differential equations (ODEs) were introduced by Dutt, Greengard and Rokhlin. It was shown that SDC methods can achieve arbitrary high order accuracy and possess nice stability properties. The methods are based on low order integration, such as forward Euler or backward Euler, and are able to handle stiff and non-stiff terms in the ODEs. In this paper, we consider using high order Runge-Kutta (RK) methods in the prediction and correction steps of SDC methods. The distribution of quadrature nodes are assumed to be uniform and the corresponding local truncation error analysis is given. The smoothness of the error function, which can be measured by the discrete Sobolev norm, is a crucial tool in our analysis. The expected order of accuracy are demonstrated through several numerical examples. Superior numerical stability and accuracy regions are observed when high order RK methods are implemented within SDC methods.

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MS63

Hierarchical Reconstruction for Discontinuous Galerkin Methods on Unstructured Grids with a Weno Type Linear Reconstruction

The hierarchical reconstruction is applied to discontinuous Galerkin method on the two-dimensional unstructured grids. We explore a variety of limiter functions used in the construction of piecewise linear polynomials. We show that due to the abrupt shift of stencils, the use of center biased limiter functions is essential in order to recover the desired order of accuracy. Furthermore, we develop a WENO type linear reconstruction in each hierarchical level. Numerical computations for scalar and system of nonlinear hyperbolic equations are performed. We demonstrate that the hierarchical reconstruction can generate essentially non-oscillatory solutions while keeping the resolution and desired order of accuracy for smooth solutions.

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MS64

Advances and Challenges in the Simulation of Field-Theoretic Models of Complex Fluids

In field-theoretic polymer models the particle-particle interactions of the molecular approach are replaced by interactions between the particles and one or more fluctuating fields defined everywhere in the domain of interest. This upscaling is achieved formally via the introduction of functional integrals and offers great flexibility for different levels of coarse-graining and model building. We will review here some basic field-theoretic models for inhomogeneous polymers and discuss recent numerical advances in the solution of these models both in the self-consistent, mean field approximation and in the presence of a processing flow and we will point also to some of the remaining challenges.

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MS64

Complex Particles and Fluids

I will discuss mathematical models of systems of particles suspended in fluids when the configuration space of the particles is nontrivial.

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MS64

An Overview of Complex Fluids for this Minisymposium

In this lecture I will give an overview of the broad areas covered in this minisymposium, then turn to some of the most recent issues of interest in my collaborations. These issues range from the phenomena we have identified through large-scale simulations, to asymptotic and geometric analysis of these phenomena in special limits, to open mathematical problems.

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MS64

Variational Approaches in Complex Fluids

Not available at time of publication.

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MS65

Supercavitating Flow Around Hydrofoils: The Method of Automorphic Functions

In the framework of the Tulin single spiral vortex model supercavitating flow around hydrofoils is analyzed. The flow domain is conformally mapped into a circular multiply-connected domain. To reconstruct the actual form of the conformal map it is needed to solve two Riemann-Hilbert problem of the theory of automorphic functions (one of them with a discontinuous coefficient). Its solution is found in a form that avoids the solution of the Jacobi inversion problem.

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MS65

New Ideas in Numerical Conformal Mapping of Multiply Connected Domains

By comparison with techniques for conformally mapping simply connected planar regions, the study of conformal maps between multiply connected regions has received much less attention. Mathematically, the problem is more challenging owing to the problem of determining the conformal moduli of multiply connected domains. This talk will survey some new ideas in this area.

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MS65

Conformal Mappings to Multiply Connected Circular Domains

An important canonical class of multiply connected domains is the class of circular domains whose boundaries are all circles. This talk will survey methods for the explicit construction of conformal mappings between arbitrary multiply connected domains and their conformally equivalent circular domains.

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MS65

Computing with Analytic and Harmonic Functions

on the Unit Disk

There are many tools for computing with analytic functions on the unit disk, including FFT, least-squares fitting on the boundary, Cauchy integrals discretized by the trapezoid rule, and the barycentric interpolation formula. From this have sprung special methods associated with names including Lyness and Delves, Luck and Stevens, and Squire and Trapp. I am attempting to bring order to this important and fundamentally easy material with a new book called "Neoclassical Numerics". This talk will outline the findings of chapter 1 of that book. ...plus a pointer to

chapter 2, which is about harmonic as opposed to analytic functions. The connections are very close, even if the standard formulations sound quite different.

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MS66

Adjoint Based Optimization and Adaptivity for Multiphysics Problems.

We present an adjoint based approach to improve the accuracy of large scale multiphysics optimization problems using adaptivity. Both error estimators of output functionals and associated sensitivities are calculated through a common adjoint formulation. Mesh refinement is thereby targeted to reduce numerical errors in the optimization problem. We demonstrate the utility of our integration through a numerical example in Sandia's Sierra Mechanics framework in which various complexities of adjoint implementations and adaptivity are addressed.

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MS66

High-Level PDE Software for Thermal Convection

While high-level software such as Sundance allows users to specify variational problems and assemble algebraic systems efficiently and abstractly, finding solver strategies presentschallengings. We will explore implementin various iterative strategies for the Benard convection problem. These include iterating between flow and temperature equations, a fully coupled Newton strategy, and physics-based preconditioner of the flow equations. We will conclude with observations about what mathematical results may be needed to study how to precondition coupled systems.

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MS66

Combining Implicit Time Integration and Spatial Adaptivity in MHD Simulations

Computational magnetohydrodynamics is demanding due to the wide range of spatial and temporal scales and strongly anisotropic and nonlinear effects due to self-generated or external electric and magnetic fields. These challenges can be addressed by using implicit time integration to accurately step over the fastest time scales and adaptive mesh refinement to enhance resolution of fine spatial features in the solution. Difficulties associated with combining the two approaches strategies for overcoming them will be discussed.

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MS66

Parallel Adaptive Solution of Mantle Convection Problems

Mantle convection is the principal control on the thermal and geological evolution of the Earth. It is central to our understanding of the origin and evolution of tectonic deformation, the evolution of the thermal and compositional states of the mantle, and ultimately the evolution of the Earth as a whole. Mantle convection simulation is an important driver for petascale computing, due to the wide range of length and time scales involved. Our goal is to conduct high resolution mantle convection simulations that can resolve thermal boundary layers and faulted plate boundaries, down to 1 km scales. To enable this (local) resolution, we are developing *Rhea*, a new generation mantle convection code incorporating parallel adaptive mesh refinement/coarsening algorithms designed to scale to hundreds of thousands of processors. We discuss parallel performance on *Ranger*, the new 500 Teraflops system at TACC.

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MS67

A Viscoelastic Timoshenko Beam with Dynamic Impact

We consider the dynamic frictionless viscoelastic Timoshenko beam (of Kelvin-Voigt type) equation, based on the complementarity conditions arising from the Signorini contact conditions. The left end of the beam is assumed to be clamped horizontally and the right end of the beam can contact a perfectly rigid obstacle. The existence of solutions is discussed and energy balance is investigated. Employing time discretization and Galerkin approximation, we compute numerical solutions which support the idea that the energy losses in the limit are equal to the losses due to viscosity

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MS67

Corner Bifurcations in Impacting Systems

Impacting problems lead naturally to non-smooth dynamical systems, the behavior of which depends can be studied in terms of non-smooth maps and their bifurcations. I will show in this talk that a variety of impacting problems, including cam devices, non-smoothly forced problems, Newton's cradle type systems and multiple body impacts can be studied in terms of discontinuous piecewise linear maps. These display extraordinarily rich dynamics when the map discontinuity interacts with the limit sets (fixed points and periodic cycles) of the system in (so called) corner bifurcations. We see period-adding and related routes to chaos as well as Farey sequences and multiple impacting states. I will develop the thoery of this behavior in this talk and then give some experimental results where it is seen in practice.

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MS67

Existence and Approximation Results for a Class of Dynamic Unilateral Contact Problems

This lecture will present a study of an interaction law coupling dynamic unilateral contact, adhesion and friction between viscoelastic bodies. The variational formulations of this class of problems will be given as systems of implicit inequalities which describe the bulk and the surface behaviors, including a parabolic variational inequality which describes the evolution of the intensity of adhesion. The existence of solutions will be investigated by using an incremental approach and a fixed point method.

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MS67

Energy Balance for Viscoelastic Impact with or without Friction

An energy balance of an elastic or viscoelastic body is where the energy of the body can be accounted for through viscous or similar losses, but not due to impact. One of us has shown that for viscoelastic bodies in frictionless contact, that there is an energy balance. More recently, we have shown an energy balance for a viscoelastic body in dynamic contact with the regularized Coulomb friction law of Kuttler and Shillor. The essential technique used to do this comes from "differentiating" a variational inequality. As a side effect, the maximum dissipation property of Coulomb friction is shown for viscoelastic bodies in dynamic contact.

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MS68

Mathematical Modeling of DNA Microarray Data: From Discovery of Patterns to Discovery of Molecular Biological Mechanisms

I will describe matrix and tensor models of DNA microarray data, where the mathematical variables, patterns uncovered in the data, correlate with activities of cellular elements. The operations, such as data reconstruction in subspaces of selected patterns, simulate experimental observation of the correlations and possibly also causal coordination of these activities. These models may form the basis of a future where molecular biological systems are modeled and controlled as physical systems are today.

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MS68

Life at Low Molecule Number

Transient molecular signals occur in microdomains that are typically neither well mixed nor in equilibirum. The number of molecules is often so small that large fluctuations occur. As a consequence, knowing the spatial organization of the molecular components is essential in understanding cell signaling pathways. We are using Monte Carlo computer simulations that incorporate realistic 3-D geometries to explore the subcellular architecture and physiology of neurons and synapses.

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MS68

Nonlinear Fokker-Planck Equations and Hybrid Systems

I will describe some of the mathematical models of systems consisting of microscopic particles interacting with fluids. These models are nonlinear Fokker-Planck equations coupled to fluid equations. They can be seen in the larger context of stochastic particle models actively coupled with fluids, forming stochastic systems, nonlinear in the sense of McKean. Patterns arise in the limit of high concentration of particles. The characterization of the patterns for complex particles, and the dynamics associated to nontrivial patterns for simple particles are subjects of current interest.

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MS68
Mathematics Amongst the Biomolecules

Modern developments in biology are revealing extraordinary dynamical complexity at the molecular level: many components, even more states, intertwined feedbacks, multiple time-scales. Bologists are turning to mathematicians for help in trying to understand such systems. Will mathematics continue to be as "unreasonably effective" in the molecular sciences as Eugene Wigner found it to be in the "natural" sciences? The answer to this may change the way we think about both biology and mathematics.

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MS69
Methods for Multilingual Text Analysis

Not available at time of publication.

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MS69
Uncertainty Quantification for Sparse Data Problems

The uncertainty quantification community has developed a robust suite of methods to solve numerical problems with deterministic parameters modeled as random variables. In this talk, Paul Constantine and I will review some of their methods and investigate a few possibilities with algorithms such as LSI and PageRank.

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MS69
Matrix Factorization Techniques for Collaborative Filtering and the Netflix Prize

Not available at time of publication.

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MS69
Computing Approximate Pagerank Vectors By Basis Pursuit Denoising

The PageRank eigenvector problem involves a square system Ax = b in which x is naturally nonnegative and somewhat sparse (depending on b). We seek an approximate x that is nonnegative and extremely sparse. We experiment with an active-set optimization method designed for the dual of the BPDN problem, and find that it tends to extract the important elements of x in a greedy fashion.

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MS70
Adaptive Mesh Refinement for Multi-Material Volume-Tracking with Moment-of-Fluid Method

A novel adaptive mesh refinement (AMR) strategy based on Moment-of-fluid (MOF) method for volume-tracking evolving interface computation is presented. Moment-of-fluid method is a new interface reconstruction and volume advection method using volume fraction as well as material centroid. The mesh refinement is performed based on the error indicator, the deviation of the actual centroid obtained by interface reconstruction from the reference centroid given by moment advection process. Using the AMR-MOF method, the accuracy of volume-tracking computation with evolving interfaces is improved significantly compared to other published results. The effectiveness and efficiency of AMR-MOF method is demonstrated with classical test problems, such as Zalesaks disk and reversible vortex problem. The comparison with previously published results for these problems shows the superior accuracy of the AMR-MOF method over other methods.

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MS70
A Multimaterial Radiation Diffusion Solver for ALE with AMR

We present a implementation of the multimaterial radiation diffusion solver on an ALE (arbitrary Lagrangian-Eulerian) mesh with AMR (adaptive mesh refinement). We will discuss the discretization of the diffusion operator. The implicit integration uses Newton's iterations with Schur's complement preconditioning. The solver's time step size determined by the quickness of nonlinear convergence. The design of the multimaterial support allows the solver to work as an optional plug-in physics module to the main code.

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MS70
Lagrangian Models and Remapping Algorithms for 2D Multi-Material ALE Methods

We will present 2D numerical algorithms for multi-material arbitrary Lagrangian-Eulerian (ALE) methods. We will focus on the Lagrangian and remapping stages generalized for multi-material fluid flows. Results for several closure models for mixed cells in the Lagrangian solver will be presented. We will describe our remapping method interpolating fluid quantities onto smoothed mesh, based on mass fluxes between neighboring cells, and propagation of fluid quantities with these fluxes.

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MS70
ALE with Automatic Reconnection Via Voronoi Diagram

We developed a 2D-ALE code on polygonal mesh for which the rezone strategy can change connectivity. For each rezone step a Voronoi mesh generator provides a new polygonal mesh from a cloud of generators; allowing the connectivity to evolve, following the fluid flow. A remapper conservatively projects information onto the rezoned mesh. We will present numerical examples on several classical hydrodynamics test cases.

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MS71
Dynamic Supernodes in Sparse Cholesky Update/downdate of Active Set Methods

Active set methods in optimization often need the update or downdate of a Cholesky factorization after a low rank change in the matrix. To achieve efficient computer implementations in a sparse matrix setting, supernodes should be exploited. Conventional supernodes are unsuitable when low rank modifications are made to the matrix since supernodes merge and split during an update/downdate. We discuss non-conventional dynamic supernodes with performance competitive to conventional supernodes, while being well-suited to active set methods.

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MS71
Trust-Search Methods for Unconstrained Optimization

Recent research on interior methods has re-emphasized the role of sequential unconstrained optimization for the solution of very large nonconvex problems We focus on the numerical linear algebra associated with a class of"trust-search" methods that combine the best features of line-search and trust-region methods for unconstrained optimization.

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MS71
Block Preconditioners for Saddle Point Linear Systems

Saddle point linear systems arise in a variety of constrained optimization problems. When these systems are very large and sparse, iterative methods must be used to compute a solution. The challenge is to derive and apply preconditioners that exploit the properties and the structure of the given discrete operators, and yield fast convergence while imposing reasonable storage requirements. In this talk I will provide a survey of block preconditioners and discuss their spectral properties, bounds on convergence, and computational advantages and disadvantages. We will look at a variety of such techniques: Schur complement based approaches, constraint preconditioners, and augmentation methods.

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MS71
Multilevel Preconditioning for Large-scale Nonconvex PDE-constrained Optimization

We propose an algebraic multilevel preconditioning technique using maximum weighted matchings for nonconvex optimization problems to be used in interior point methods. The preconditioning approach for the symmetric indefinite Karush-Kuhn-Tucker systems is based on maximum weighted matchings and algebraic multi-level inverse-based incomplete LBL^T factorizations. The largest nonconvex optimization problem from three-dimensional PDE-constrained optimization with the multilevel preconditioning approach has more than 30 million state variables and hundred of thousands control variables with both lower and upper bound.

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MS72
Stochastic Analysis of Electrostatic MEMS

We present a stochastic collocation framework to quantify the effect of random input parameters on electrostatic MEMS, modeled using stochastic PDEs. The main idea is to adaptively decompose the multi-dimensional space of random inputs into subdomains, and then to employ a sparse grid interpolation procedure within each subdomain. This approach is well suited to handle discontinuities in the random domain. Numerical examples are presented to demonstrate the accuracy and efficiency in computing the required statistics.

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MS72

Efficient Particle Filtering Algorithms for Data Assimilation

Particle filter is an important method for nonlinear sequential data assimilation. However, its usage is severely limited due to the relatively large computational effort resulted from the requirement of sufficiently large ensemble of particles for accurate approximation of distribution functions. Here we present a particle filter method by taking the advantage of general polynomial chaos (gPC) methodology, which allows one to utilize large number of particles. The distribution of the model states can be well approximated and the weights of the particles can be calculated more accurately. Numerical examples are provided to verify the convergence property of the new method.

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MS72

A Polynomial-Chaos Based Approach for Parameter Estimation

The polynomial chaos method has been shown to be considerably more efficient than Monte Carlo in the simulation of systems with a small number of uncertain parameters. We discuss a new approach for parameter estimation in a Bayesian framework which uses the polynomial chaos framework to represent the uncertainty in the system response. The methodology is applied to estimate the uncertain mass and inertia of a vehicle dynamic model.

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MS72

Efficient Numerical Simulations for Stochastic Maxwell Equations with Applications in Photonic Crystal Spectrometer Design

We propose a new stochastic model for general spatially incoherent sources. The model naturally incorporates the incoherent property and leads to stochastic Maxwell equations. Fast numerical methods based on Wiener Chaos Expansions (WCE), which convert the random equations into system of deterministic equations, are developed. We apply the model and method to photonic crystal spectrometer design and the new methods can achieve 2 order of magnitude faster computation time over the standard method used in applications.

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MS73

Cython: A Python to C Compiler

High level languages such as Python enable rapid prototyping and easy experimentation, but often lack the speed necessary for serious scientific computing. Cython, based on Pyrex, allows python-like code to use C/C++ libraries and C/C++ data types/structures directly. This lets one write highly optimized routines using low level operations and easily create Python wrappers of C/C++ libraries. We will explain how Cython works, and demonstrate it via some simple examples.

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MS73

NiPy: Neuroimaging in Python

We describe an open source package for analysing functional Magnetic Resonance Imaging (fMRI) data called Neuroimaging in Python (NiPy). The purpose of this project is twofold: first it provides tools developed by a broad group of international collaborators for fMRI data analysis. Second, it is structured as a set of components with well defined interfaces for each step of a typical fMRI workflow, to enable novel algorithmic and analysis approaches to be developed and integrated.

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MS73

Exact Linear Algebra in Sage

As a building block in numerous scientific computations, exact linear algebra in sage has to compose with both efficiency and genericity. For this purpose, it relies on a combination of proper implementations, some features of the LinBox and IML libraries, and the numerical BLAS routines. We will first present the overall organization of these implementations in Sage, and then illustrate it with a few applications where SAGE sets the state of the art efficiency for these problems.

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MS73

Investigating Flight Behaviour of Fruit Flies Using Multi-camera Tracking

Much of what we know about the visual guidance of flight, aerial pursuit, olfactory search algorithms and control of aerodynamic forces is based on experiments tracking insects in flight. We created a new, automated insect tracking system capable of tracking over large, behaviorally-relevant spatial scales with high resolution. The system uses multiple digital video cameras connected to a cluster of computers, controlled in real time by an in-house, Python based software system.

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MS74

An Enhanced Macroscopic Closure Approximation to the Micro-Macro Fene Models for Polymeric Materials

Not available at time of publication.

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MS74

Direct and Inverse Methods for Diffusive Transport in Biological Fluids

We study the diffusive behavior of micron-sized beads in biological fluids in conjunction with particle tracking experiments. The model consists of a generalized Langevin equation (GLE) with a memory kernel. The Fluctuation-Dissipation theorem yields the connection between the random force and the memory kernel. We study the direct and inverse characterization problems using numerical tools and methods developed for noisy time series.

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MS74

Angular Momentum Transport in Complex Fluids

When dyes are dissolved in nematic liquid crystals, the light intensity required for the optical Freedericksz transition can be dramatically decreased. This is due to the torque exerted by the dye on the liquid crystal. The dye molecules absorb light energy and rotate; torque balance is mediated by angular momentum transport from the cell walls via shear flow generated by the rotation. We present a model which accounts for the transport of angular momentum caused by singular vortices present in these complex fluids. The singular vortices generate flow, and are transported by the flow which they generate. For simple fluids, the distribution of vorticity satisfies the biharmonic equation in the Stokes limit, which can be solved analytically. In the case of the non-Newtonian fluids, such as liquid crystals, Leslie-Ericksen continuum theory is used to describe the interactions between the rod-like molecules.

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MS74

Numerical Simulations of Rigid-rod Polymer Hydrodynamics

We study the behavior of nematic rigid-rod polymers confined between moving plates using the kinetic model equation coupled with Navier-Stokes equation. Numerical simulation results about the correlations among polymer anchoring conditions, structure formation, stress, and hydradynamic feedback will be shown.

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MS75

Interior Point Methods for Mixed-integer Nonlinear Conic Programming

Recent studies show that interior-point methods are highly efficient on large-scale nonlinear and cone programming. However, their inability to warmstart has largely limited their applications to problems with continuous variables. In this talk, we will present a unified interior-point framework for efficiently handling mixed-integer nonlinear programming problems with cone constraints and provide numerical results.

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MS75

Interior Point Methods for Simulating Multibody Systems

The dynamic rigid multibody contact problem is concerned with the motion of several rigid bodies with frictional contacts. Modern time-stepping schemes for simulating such systems require the solution of a linear complementarity problem at each step. In the absence of friction the LCP is monotone and can be solved in polynomial time by interior point methods (IPMs). We investigate the performance of IPMs in the presence of small to moderate friction.

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MS75

Interior Point Methods for Protein Image Alignment

We present a new approach for aligning families of 2D-gel images arising in proteomics which uses the information contained in the whole family for creating an ideal gel and determining transformations that optimally align the images. The ideal landmarks and the coefficients defining the transformations are obtained by solving a large-scale quadratic programming problem. We assess the numerical performance of various interior-point algorithms on some large scale image alignment problems.

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MS75

The Redevelopment of SeDuMi

We present an object-oriented open-source platform for rapid porting, prototyping and development of interior-point method algorithms in C++, targeted for SMP architecture. YAS is designed to allow easy extensions of IPM beyond the symmetric cone programming. Currently within the platform, basic long-step, predictor-corrector, and Nesterov's asymmetric primal-dual methods are implemented. YAS provides SeDuMi-like interface for MATLAB and Octave, with the capability of building standalone applications.

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MS76

Compact Upwind Second Order Scheme for Eikonal Equation

A Compact Upwind Second Order Scheme is presented.The scheme is based on Fast Sweeping Method and an interesting phenomenon: the gradient of a smooth solution obtained by first order Fast Sweeping Method is still first order.An idea for a possible proof of this interesting phenomenon of distance function is proposed.Numerical examples for first order gradient and second order fast scheme will be given. (joint work with J.D. Benamou and H.K. Zhao)

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MS76

High Order Methods for the Eikonal Equation

The fast sweeping method combines alternate direction Gauss-Seidel iterations with a local solver. Ideally, for the Eikonal Equation the local solver will: 1) depend only smaller arrival times (causality); and 2) use a fixed grid (Eulerian method). The first requirement is necessary for fast global convergence of the fast sweeping method and efficient local solvers require (2). Previously methods have been developed that weaken conditions (1) or (2). Weakening (1) dramatically increases the number of global iterations, while weakening (2) substantially increases the cost of the local solver due to local iterations and high dimensional interpolation. In this talk we develop high-order local solvers that that are both causal and Eulerian. We demonstrate the efficiency of this technique with a number of 2D examples.

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MS76
Weighted PowerENO Sweeping Methods for Static Hamilton-Jacobi Equations

First order fast sweeping methods are well developed and efficient algorithms for the approximation of the viscosity solution of static Hamilton-Jacobi equations. In this research work we construct fifth order accurate sweeping methods based on the Weighted PowerENO scheme developed by Serna and Qian for time dependent Hamilton-Jacobi equations. Numerical examples including eikonal equations show that our fifth order methods achieve high order accuracy in smooth regions and sharp resolution of discontinuities of derivatives.

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MS76
Discontinuous Galerkin Fast Sweeping Methods

In this presentation, I will talk about our recent progress on developing high accuracy fast sweeping methods based on discontinuous Galerkin (DG) finite element local solver. A novel strategy is developed to combine the compact DG discretization with the causality of the Eikonal equations. Good accuracy and fast convergence speed will be shown via numerical examples.

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MS77
Systems Genetics

We integrated genetic interaction data and molecular interaction data to model the transcription network controlling cell differentiation in yeast. Genetic interactions were inferred from linear decomposition of gene expression data and were used to direct the construction of a molecular interaction network mediating these genetic effects. The network model predicted quantitative gene expression profiles and precise phenotypic effects for novel combinations of mutations. Multiple predictions were tested and verified.

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MS77
Integrating DNA Microarray Data From Different Studies Using Higher-Order Singular Value Decompositions

We compare the N-mode SVD and the parallel factorization (PARAFAC) in integrating DNA microarray data from three cell cycle time courses, under different oxidative stress conditions. Each decomposition formulates the data tensor as a linear superposition of different rank-1 subtensors. We show that significant subtensors of both decompositions represent independent biological programs or experimental phenomena. The N-mode SVD also uncovers previously unrecognized subtle yet robust effects of the oxidative stress conditions on the cell cycle.

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MS77
New Methods for Analyzing High Throughput Sequence Data

High-throughput sequencing has undergone remarkable increases in efficiency over the past few years. We have developed techniques to process and interpret such data. There are two main areas we have tried to address with our software: (1) mapping of short reads to reference sequences and (2) improving our ability to estimate the sequence of each read.

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MS77
Information Aspects of Molecular Measurement Technologies

DNA microarrays enable the high throughput measurement of hunreds of thousands of nucleic acid binding reactions in a single assay. Microarrays have evolved over recent years to address a range of genomic measurement tasks. The development of array based genome wide DNA copy number profiling has opened the door to a variety of other applications. Manufacturing techniques that enable flexible design of probes and complete arrays in various sizes complete the picture to yield a varsetile measurement platform. I will describe the use of microarrays in several research projects, including studies of the time of replication in S phase, studies of chromosomal aberrations in

cancer and of copy number vaiations (CNVs) in normal populations. The talk will emphasize some of the computational and statistical aspects of flexible designs and of specific applications.

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MS78

Contact with Slip and Friction in Multi-Material Arbitrary Lagrangian Eulerian Formulations

An extended finite element formulation is presented for large deformation contact with slip and friction. Example calculations are compared to the Lagrangian solutions obtained from LS-DYNA, an explicit finite element program.

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MS78

Solid Fragmentation Modeling with the Multi-Material Implementation in NIF ALE-AMR

The NIF ALE-AMR code is capable of modeling multi-material solids using a volume of fluid approach. This multi-material approach can also be naturally extended to cover fragmentation by tracking void formation and growth in solid material cells. We present numerous NIF ALE-AMR simulations to validate this approach, and some interesting results that have been obtained with these methods.

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MS78

Spherical Geodesic Mesh Generation

For calculations on spherical meshes, solution-mesh coupling may lead to errors and symmetry-breaking. Although the underlying differencing scheme may be modified to rectify this, the differencing scheme may not be accessible. This documents the use of spherical geodesic meshes (connected, concentric, triangularized spherical surfaces) to mitigate solution-mesh coupling. Using an ALE hydrocode, results show that while symmetry is broken on traditional meshes, symmetry is sometimes improved on spherical geodesic meshes.

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MS78

A Second Order, Cell-centered Lagrangian Scheme for Multidimensional (2D and 3D) Compressible Flows and its Application to ICF Direct Drive Simulation

We present a new unstructured cell-centered scheme for multidimensional Lagrangian hydrodynamics. The vertex velocities and the numerical fluxes through the cell interfaces are evaluated in a consistent manner due to a nodal solver. This solver is contructed such that momentum and total energy conservation are ensured. In addition, a semi-discrete entropy inequality is provided. The time and space second order extension utilizes the methodology of linear Generalized Riemann Problem in the acoustic approximation.

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MS79

Compressive Wave Computations

We propose to solve time-dependent wave equations in an embarrassingly parallel way by precomputing a small set of eigenfunctions chosen at random, and synthesizing the solution by solving an ell-1 problem remindful of compressed sensing. In one spatial dimension, if the solution has the right sparsity properties, the complexity of this method is linear with log factors in the data volume—where a timestepping-based method would be quadratic and a Helmholtz-based method would be cubic. In seismology, this approach sheds new light to the memory overhead problem in reverse-time migration. The justification of performance involves a new Strichartz-like estimate for wave equations in BV media. Joint work with Gabriel Peyre.

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MS79

A Parallel Upscaling Technique for Elastic Wave Propagation

Modeling elastic wave propagation in the earth sciences often involves reconciling data from multiple scales. However, computational limitations often require the use of a grid that is coarse relative to finer scale features of the domain. Operator upscaling adequately deals with this issue by imparting fine scale accuracy to the coarse solution. Further, operator upscaling has the advantage that it is particularly susceptible to parallelization. I present a fully parallel upscaling elastic wave propagation code and present numerical experiments that demonstrate the performance of the parallel code.

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MS79

Upscaling Non-Darcy Flow for Preferential Flow

We consider upscaling of non-Darcy flow in heterogeneous porous media. Our approach extends the pressure-based numerical homogenization procedure for linear Darcy flow due to Durlofsky to the nonlinear case. The effective coefficients are not constants but rather mildly varying functions of prevailing gradients of pressure. The upscaled model approximates the fine grid model accurately and, in some cases, more accurately than what is expected for Darcy flow; this is due to the non–Darcy effects which suppress heterogeneity. We provide comparisons of alternative approaches as well as consider several variants of numerical realizations of the non–Darcy flow model. Numerical results show effectiveness of the upscaling procedure. This is joint work with Cristiano Garibotti.

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MS79

Superpositions of Gaussian Beams

Gaussian beams are approximate high frequency solutions to PDEs which are concentrated on a single ray through space-time. More general solutions that are not necessarily concentrated on a single ray can be obtained from a superposition of Gaussian beams. Since Gaussian beam superpositions provide a global approximate solution, this solution gives a valid description of the wave field near caustics, where traditional ray based methods fail. In geophysical applications, Gaussian beam superpositions have been used to model the seismic wave field, and for seismic migration. We will discuss some recent developments in Gaussian beams.

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MS80

An Efficient Monte Carlo Method Using Sensitivity Derivatives

We investigate efficient numerical algorithms for the optimal impedance factor identification of a noise radiation problem. We treat the acoustic wavenumber as a random variable. As result, the state equation is a stochastic Helmholtz equation. An efficient Monte Carlo numerical algorithm will be implemented to evaluation the expected cost function. Numerical results indicate significant noise reduction.

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MS80

Predictability and Reduced Order Modeling in Stochastic Reaction Networks

Spectral methods combined with reduced order modeling are used for the dynamical analysis and predictability of stochastic reaction networks described by a chemical master equation. Namely, we explored polynomial chaos expansions with Karhunen-Loeve decomposition of stochastic processes to quantify parametric as well as intrinsic uncertainties in stochastic dynamical systems. This methodology along with adaptive multi-resolution analysis has been applied to bistable systems of biophysical interest.

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MS80

Discontinuity Detection in Stochastic Computations

Stochastic variants of deterministic models (differential equations) arising in engineering problems can have several variables depending on the nature of the random inputs. Polynomial methods are often used to approximate stochastic solutions to such problems. However, stochastic solutions to these problems sometimes contain discontinuities in the corresponding random variable space, adversely affecting the solution. This talk expands the use of the polynomial annihilation local edge detector first proposed by Archibald, Gelb and Yoon in 2005 to locate discontinuities in such multi-dimensional data. Prior knowledge of jump locations for these problems can be helpful in increasing the accuracy of the final solution.

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MS80

Elliptic Problems with Non-Gaussian Inputs: A New Method

We propose a simple and effective numerical procedure for solving elliptic problems with non-Gaussian random coefficients, assuming that samples of the non-Gaussian random inputs are available from a statistical model or experimen-

tal data. A Karhunen-Loève (K-L) expansion is employed to reduce the dimensionality of random inputs. Using a density estimation technique, we obtain the marginal probability density functions (PDFs) of the random variables in the K-L expansion, based on which we define an auxiliary joint PDF. We then implement the generalized polynomial chaos (gPC) method via a collocation projection according to the auxiliary joint PDF. Based on the observation that the solution has an analytic extension in the parametric space, we ensure that the polynomial interpolation achieves a point-wise convergence in the parametric space regardless of the PDF, where the energy norm is employed in the physical space. Hence, we can sample the gPC solution using the joint PDF instead of the auxiliary one to obtain the correct statistics. We also implement Monte Carlo methods to further refine the statistics using the gPC solution for variance reduction. Numerical results are presented to demonstrate the efficiency of the proposed approach.

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MS81

Interactive Parallel Computing and Distributed Arrays in Python

In this talk, I will describe efforts to develop an open-source architecture for parallel computing in Python. This architecture 1) has high-level interfaces that supports rapid development, 2) enables all aspects of parallel computing to be performed interactively and 3) supports many different models of parallel computing. The focus of this talk will be on recent work implementing distributed arrays within this architecture.

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MS81

Distributed Computing with Sage

DSage or Distributed Sage, is a framework for easily running and managing distributed computational projects. It is designed to allow many computers in a heterogeneous environment to pool their resources in attacking a problem. DSage is most useful for problems that are highly parallelizable and do not require communication between different nodes. We will give a few demonstrations of DSage in action and outline how DSage has been successfully used in mathematical research previously.

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MS81

Software Components for Scientific Computing

In my laboratory we use computational models for simulating molecular interactions. One of the challenges we face is the integration and interoperation of computational techniques from a wide variety of scientific disciplines. We present a component-based software development strategy centered on Python. We describe several software components including our visual programming component Vision and illustrate their integration. Concepts such as distributed computing and web-services will be touched upon as well.

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MS81

PyTrilinos: A Python Interface to Parallel, Object-Oriented Solver Packages for Scientific Computing

The Trilinos Project at Sandia National Laboratories is a collection of several dozen interoperable, object-oriented solver packages. These packages span serial and parallel implementations; linear algebra services for dense and sparse problems; linear-, nonlinear-, and eigensolver algorithms; preconditioners; and a wide variety of tools, such as reference counted memory management, parameter lists, and load balancing. PyTrilinos is a python interface to selected Trilinos packages, explicitly compatible with NumPy, and thus interoperable with SciPy.

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MS82

Curve and Surface Segmentation Using Minimal Paths

Active contours define the desired curve or surface as minimizing a relevant energy functional. Minimal geodesics allow to find global minimum of active contour energy using Fast Marching to solve Eikonal equation. This talk will focus on various segmentation methods in this framework. We developped recently a new approach in 2D and 3D through a set of minimal paths by adding automatically and iteratively keypoints that distribute uniformly on the boundary we wish to find.

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MS82

Unsupervised Feature Balancing Multi-phase Segmentation

In multiphase segmentation, typically there is an instability issue associated with choosing the number of phases which is needed to segment the image appropriately. In this talk, we propose a new variational functional for an unsupervised multiphase segmentation, by adding scale information of each phase. The minimum of the functional automatically chooses the reasonable number of phases to be detected as well as identify each phase. We explore a fast pixel-wise decision process for the proposed functional and present number of experiments showing the robustness of this method.

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MS82

Self-Repelling Snakes for Topology-Preserving Segmentation

The implicit framework of the level set method has several advantages when tracking propagating fronts (evolving contour embedded in a higher-dimensional level-set function, easily-handled topological changes), which makes it useful in a wide range of applications such that image segmentation. Nevertheless, in some applications (cortex reconstruction, etc) this topological flexibility turns out to be undesirable. Thus we propose a segmentation model based on an implicit level set formulation and on the geodesic active contours, in which a topological constraint is enforced.

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MS82

Deformable Models with Topological Preservation on Octree Grids

It is increasingly popular to represent objects on adaptive grids such as octree grids in order to save on both storage requirements and computation time. Many algorithms that were developed for regular grids have been modified for adaptive grids. This talk describes an approach to geometric deformable models on octree grids that preserves object topology. First, definitions and concepts from the theory of digital topology on regular grids are adapted for octree grids. Then the strategy developed for the topology-preserving deformable model (TDGM) is used. Results are demonstrated on both computational phantoms and human images of the pelvis and brain.

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MS83

Parameterizing Exponential Family Models for Random Graphs: Current Methods and New Directions

Let G be a random graph (typically on some finite support S), such that the log-probability of a given realization $G = g$ may be written as the inner product $\theta^T t(g) - \psi(\theta, S)$, where θ is a constant real vector of length k, t is a k-vector of real-valued functions on S, and ψ is a real-valued function depending only on θ and S. The distribution of G written in this way is said to be in exponential family form, and the vector t defines a discrete exponential family of distributions on S. Such exponential families are increasingly used as models for the structure of social networks, since they provide a highly general mechanism for parameterizing dependence among edges and are supported by a growing body of computational and inferential theory. An important and ongoing challenge within this line of research is to find principled ways of proposing vectors of graph statistics (i.e., t) which parsimoniously capture the dependence associated with particular social mechanisms. Here, I will review some current approaches to the parameterization problem, as well as an alternative based on the use of potential games. I will briefly illustrate the application of these techniques to the modeling of interpersonal relationships, and show how the respective parameterization schemes can aid in the interpretation of both new and existing models for relational data.

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MS83

Opportunistic Communications: Modelling Inter Contact Times Between Human-carried Mobile Devices

We examine the fundamental properties that determine the basic performance metrics for opportunistic communications. We first consider the distribution of inter-contact times between mobile devices. Using a diverse set of measured mobility traces, we find as an invariant property that there is a characteristic time, order of half a day, beyond which the distribution decays exponentially. Up to this value, the distribution in many cases follows a power law, as shown in recent work. This power law finding was previously used to support the hypothesis that inter-contact time has a power law tail, and that common mobility models are not adequate. However, we observe that the time scale of interest for opportunistic forwarding may be of the same order as the characteristic time, and thus the exponential tail is important. We further show that already simple models such as random walk and random waypoint can exhibit the same dichotomy in the distribution of inter-contact time as in empirical traces. Finally, we perform an extensive analysis of several properties of human mobility patterns across several dimensions, and we present empirical evidence that the return time of a mobile device to its favorite location site may already explain the observed dichotomy.

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MS83

Modeling Social and Economic Exchange in Net-

works

The study of bargaining has a long history, but many basic settings are still rich with unresolved questions. In particular, consider a set of agents who engage in bargaining with one another, but instead of pairs of agents interacting in isolation, agents have the opportunity to choose whom they want to negotiate with, along the edges of a graph representing social-network relations. Motivated by the division of power within social groups more generally, the field of network exchange theory has developed a large body of experimental evidence for the way in which people behave in such network-constrained bargaining situations, and it is a challenging problem to develop models that are both mathematically tractable and in general agreement with the results of these experiments. We analyze a natural theoretical model based on the work of Cook and Yamagishi in network exchange theory, which can be viewed as a direct extension of the well-known Nash bargaining solution to the case of multiple agents interacting on a graph. While this generalized Nash bargaining solution is surprisingly effective at picking up even subtle differences in bargaining power that have been observed experimentally on small examples, it has remained an open question to characterize the values taken by this solution on general graphs, or to find an efficient means to compute it. Here we resolve these questions, characterizing the possible values of this bargaining solution, and giving an efficient algorithm to compute the set of possible values. Our results exploit connections to the structure of matchings in graphs, including decomposition theorems for graphs with perfect matchings.

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MS83
Network Formation and Communication

We study a model of network formation in the context of information aggregation. Agents receive private information about a payoff-relevant state variable. Before agents make individual decisions, signals can be credibly communicated to other agents. The choices about with whom to communicate are represented by the formation of costly binary links, for which mutual consent is required. We partially characterize pairwise stable networks, and show that the model often fails to admit them. A variety of alternatives are discussed and compared to the structure of socially efficient network structures.

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MS84
Modeling of Epileptic Seizures using Tensor Analysis

We introduce mathematical models based on multi-modal data construction and analysis with a goal of understanding epilepsy seizure dynamics and developing automated/objective approaches for the analysis of large amounts of scalp electroencephalogram (EEG) data. We demonstrate that rearranging multi-channel EEG signals as third-order tensors and analyzing these tensors using multiway models give promising results in terms of identifying seizure origins as well as marking seizure periods.

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MS84
Harmonic Analysis, Parallel Factor Analysis, and a Theorem by Sylvester

In this talk we consider three seemingly different problems: harmonic analysis, the decomposition of symmetric $(2\times 2\times \ldots \times 2)$ tensors in a sum of symmetric rank-1 terms, and the decomposition of quantics in a sum of powers of linear forms. We show that this is one and the same problem. It turns out that Prony's method for harmonic analysis was also derived by Sylvester.

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MS84
Tensor-CUR Decompositions For Tensor-Based Data

The tensor-CUR decomposition is a data analysis tool important when data consist of one mode that is qualitatively different than the others. The tensor-CUR expresses the original data tensor in terms of subtensors that are actual data elements and thus have natural interpretation in terms of the processes generating the data. We employ this approach in the analysis and compression of hyperspectral medical image and in the reconstruction of consumer recommendation systems with missing data.

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MS84
TensorFaces: Multilinear (Tensor) Decomposition of Image Ensembles

Natural images are the composite consequence of multiple factors related to scene structure, illumination, and imaging. Multilinear algebra, the algebra of higher-order tensors, offers a potent mathematical framework for analyzing the multifactor structure of image ensembles and for addressing the difficult problem of disentangling the constituent factors or modes. Our multilinear modeling technique employs a tensor extension of the conventional matrix singular value decomposition (SVD), known as the N-mode SVD.

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MS84
Multilinear (Tensor) Independent Component Analysis

Multilinear ICA (MICA) model of image ensembles decomposes the image manifold into multiple subspaces associated with the different factors related to scene structure, illumination and imaging, which are inherent to image formation. MICA is a nonlinear multifactor model that generalizes ICA. MICA model of image ensembles learns the statistically independent components of the different image formation factors. Whereas ICA employs linear (matrix) algebra, MICA exploits multilinear (tensor) algebra.

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MS85

Convection, the Mean Circulation, and Convectively-Coupled Waves in an Intermediate Complexity Moist Atmospheric Model

We present results from a simplified moist general circulation model, designed to bridge the gap between simple theoretical models and more comprehensive climate models. We summarize some recent results derived with this model on the strength of the tropical overturning circulation with increased global temperatures, and mechanisms determining the strength and speed of equatorial Kelvin waves, which dominate the variability in the model tropics.

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MS85

Equatorial Convectively Coupled Waves in a Simple Multicloud Model

Linear stability analysis for the multicloud models of Khouider and Majda (2006, 2007), reveal the persistence of convectively coupled waves, unstable at the synoptic scales, in agreement with the satellite–outgoing longwave radiation (OLR) spectral peaks identified by Wheeler and Kiladis (1999). The horizontal wave structure and vertical wavenumber of the unstable waves qualitatively match those of the rotating equatorial shallow water waves but with a reduced phase speed, as in the observations. More importantly, they exhibit the same self-similar front-to-rear vertical tilt in the zonal winds, temperature, and heating fields, as observed by Kiladis and co-authors. In this talk, we discuss some physical and dynamical features of these waves and present some preliminary direct nonlinear simulations using the multicloud model in a beta plane channel. The role of low-level moisture convergence and congestus preconditioning prior to deep convection are highlighted.

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MS85

The Multi-Cloud Parameterization in a High-Order GCM

We report results concerning the multicloud parameterization scheme of Khouider-Majda and its coupling to a next generation AGCM based on the spectral element method (HOMME: High-Order Method Modeling Environment). The latter is ran in a stand-alone aquaplanet mode to examine the organization of coherent convection in the simplest possible setting. Hopefully, this will help understand the role of bimodal heating in the upscale organization of equatorial wave modes and the Madden Julian Oscillation (MJO).

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MS85

Gravity Waves in Shear and Implications for Organized Convection

Moist convection generates gravity waves that may suppress or favor the formation of new, nearby convection. This phenomena is currently not well understood for cases of anisotropic, organized convection such as convectively coupled waves. Here the nonlinear effects of gravity waves interacting with wind shear are considered in a simplified model with interesting mathematical properties (conditionally hyperbolic, nonconservative PDE with conserved energy). Results suggest a key role for wind shear/gravity waves in organized convection.

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MS86

Radial Basis Functions and Vortex Methods for Atmospheric Flows

Vortex blob methods approximate a flow as a sum of many small vortices of Gaussian shape, and adaptively move the vortex centers with the flow. Gaussian radial basis functions (RBFs) do exactly the same. However, RBFs solve an exact interpolation problem — expensive but accurate — while vortex methods sacrifice accuracy for the absence of a matrix inversion. We compare the two strategies and describe a middle ground for geophysical flows on the sphere.

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MS86

Moving Vortices on A Sphere: Local Node Refinement for Radial Basis Functions

The first use of mesh-free local node refinement with radial basis functions (RBFs) is presented. The test case is the

wrap-up of two moving vortices on the sphere. The results are compared with a discontinuous Galerkin method, semi-Lagrangian method and a finite volume method. The RBF method gives error estimates that are at least an order of magnitude lower for a much lower number of nodes, while being able to take unusually large time steps.

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MS86

Adaptive Mesh Refinements for Weather and Climate Models

Adaptive Mesh Refinement (AMR) techniques are powerful tools for weather and climate models. They not only provide refined resolutions over mountainous terrain or near land-sea boundaries but also allow tracking intense storm systems. The talk will review the latest developments in AMR for weather and climate models. In particular, two block-structured approaches in cubed-sphere and latitude-longitude geometry will be compared. The examples will include tracer advection, gravity waves, baroclinic and Rossby waves and idealized cyclones.

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MS86

Modeling Space Weather

The Center for Space Environment Modeling (CSEM) at Michigan has developed the Space Weather Modeling Framework (SWMF) that integrates independently developed models into a high performance simulation tool. The SWMF models physics domains spanning from the solar corona and heliosphere to the magnetosphere, ionosphere and thermosphere of the Earth, performing a realistic Sun-to-thermosphere simulation faster than real time on today's supercomputers. We will describe the challenges of modeling space weather, current capabilities of the SWMF, and discuss for future development.

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MS87

Multiphasic Models of Cell-matrix Interactions in Articular Cartilage

Articular cartilage can be modeled as a multiphasic continuum mixture of collagen, (negatively charged) proteoglycan, and interstitial fluid with dissolved ions. Mechanical and chemical variables in the local extracellular environment of cartilage strongly influence cellular metabolic activity in this tissue. In this talk, multiphasic models of cell-matrix interactions will be discussed. Solutions of micron-scale boundary value and interface problems that model in vitro experiments on cartilage explants will be presented.

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MS87

Instablities in Smectic Liquid Crystals

We use the continuum theory on smectic C liquid crystals to see the switching dynamics in a simple geometry. We prove the existence and uniqueness of traveling wave solutions and show that the dynamic model exhibits a slightly faster switching time than the static model. We also investigate the instability in smectic A liquid crystals when the magnetic field is applied in the direction parallel to the layers. When liquid crystals are confined in a slab, we derive analytic estimates for the magnetic field strength, at which the undeformed state loses its stability.

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MS87

A Double Projection Method for FENE-type Incompressible Flow

Incompressible viscoelastic flows cannot sustain longitudinal modes. Computations based upon explicit, time-split methods can introduce spurious longitudinal forces. The Double Projection Method (DPM) has been introduced for Oldroyd-B models to eliminate such stresses. Here, the DPM is extended to incompressible viscoelastic flows governed by FENE type models.

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MS87

Controllability of Complex Fluids

The controllability of complex fluids is a fundamental concept that defines some essential capabilities and limitations of the resulting materials. We study the controllability of different homogeneous flow fields of various complex fluids. The approach is largely based on the nonlinear geometric control theory.

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MS88

Legendre-Transform-Based Fast Sweeping Methods for Static Hamilton-Jacobi Equations

We propose a new sweeping algorithm which utilizes the Legendre transform of the Hamiltonian on triangulated meshes. The algorithm yields the numerical solution at a grid point using only its one-ring neighboring grid values and is easy to implement numerically. The scheme is shown to be monotone and consistent. We illustrate the efficiency and accuracy of the new method with several numerical examples in two and three dimensions.

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MS88

Further Results on the Complexity of Fast Sweeping Algorithms

A primary goal in most algorithms for approximating stationary Hamilton-Jacobi equations is to reduce the number of node updates that must be computed. On unstructured meshes in arbitrary dimension, we explore simple conditions on the sweep orderings which can have a large effect on the number of such updates that must be undertaken to achieve convergence. We demonstrate the results on several examples, including nonconvex Hamiltonians.

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MS88

Simplex Free Adaptive Tree Fast Sweeping and Evolution Methods for Solving Level Set Equations in Arbitrary Dimension

We introduce simplex free adaptive tree numerical methods for solving static and time dependent Hamilton-Jacobi equations arising in level set problems in arbitrary dimension. It has enough simplicity that minor variants of standard numerical Hamiltonians developed for uniform grids can be applied, yielding consistent, monotone, convergent schemes. Combined with the fast sweeping strategy, the resulting tree based methods are highly efficient and accurate. Joint work with Tom Cecil and S. Osher.

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MS88

A Few Thoughts on the Fast Sweeping Method

I will present a few thoughts that really explain the motivations behind the development of fast sweeping methods. In particular I will discuss how to unify a few derivations of the local solver from different perspectives. A few open problems will also be mentioned.

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MS89

Epigenetic Programming and Reprogramming of DNA Rearrangements

Global DNA rearrangements occur in many cells but are most exaggerated in ciliated protozoa. During development of a specialized nucleus, Oxytricha destroys 95% of its genome, severely fragmenting its chromosomes, and then sorts and reorders hundreds of thousands of remaining pieces. Understanding how the information is encoded to reorder all these pieces has been the subject of both modeling and experiments. I will show that RNA molecules provide a scaffold to program these DNA rearrangements during development, unveiling a new role for RNA, normally thought of as a passive message or intermediate in gene expression. As an example of inheritance beyond the conventional DNA genome, we demonstrate that a complete RNA cache of the parental somatic genome may epigenetically transfer information across generations, hinting at the power of RNA molecules to sculpt the information in our genomes. (reference: Nowacki et al. Nature vol. 451, p.153)

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MS89

Matrix Decompositions For Identifying Patterns of Evolution in RNA Sequences

We describe the use of singular value decomposition (SVD) in analyzing an alignment of conserved sequences. SVD simultaneously classifies the sequences into groups, and identifies characteristic sites that are unique to these groups. We show that, for an alignment of 16S ribosomal RNA sequences, the groups correspond to phylogenetic taxa, and the characteristic sites correlate with known sequence and structure motifs in the data, some of which are associated with functions like RNA- or protein-binding.

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MS89

O Stem Cell, Where Are Thou?

Human stem cell studies are difficult because many of the powerful experimental approaches that mark and follow stem cells and their progeny are impractical. Moreover, it would literally take a lifetime to follow stem cell fates prospectively. An ideal method would not require prior experimental manipulations but still allow inferences about human stem cells from birth to death. Histories are likely to be recorded within somatic cell genomes by replication errors. Therefore it should be possible to reconstruct stem cell histories by measuring the random somatic changes that accumulate within their genomes, or the genomes of their more-easy-to-identify progeny. We use a novel high-throughput approach to measure methylation patterns at certain CpG islands, and infer properties of stem cells using inference for a stochastic model of cell division and methylation changes. We will describe some of the bioinformatic and inferential problems this approach raises. Applications to cancer biology will be discussed.

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MS89

Gene Finding Algorithms in Prokaryotes and Eukaryotes Based on Stochastic Modeling

In this paper, we study the problem of predicting the genes of an organism from its genome. Our approach is probabilistic, and is based on the well-known phenomenon that the statistical distribution of the nucleotides in genic regions is quite different from that in the non-genic regions. We initially model both the gene and non-gene regions by fifth-order Markov chains, and then reduce the size of the state space using a recent method known as 4M (Mixed Memory Markov Model). This method has been validated on some bacterial genomes, and in the talk this will be discussed, as well as the extension of the method to eukaryotic (higher life form) genomes.

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MS90

Micromechanical Modeling of Fragmentation Using ALE-AMR

Fragmentation of polycrystalline materials is modeled at the grain level using single crystal plasticity with a spatially varying failure criteria using the arbitrary Lagrangian Eulerian formulation combined with automatic mesh refinement in the LLNL code ALE-AMR.

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MS90

Multimaterial ALE Method for Compressible Flows

In this talk we are interested in multimaterial flow simulations, where an interface exists between two immiscible fluids. We present new results obtained using an original coupled "ALE/interface reconstruction" method to solve hydrodynamic problems. Our method is based on a unstructured cell-centered second order Lagrangian scheme. Numerical results are used to highlight the utility of such a method over single concentration model methods, illustrated by the so-called Richtmyer-Meshkov instability problem.

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MS90

Relaxation Schemes for Non Conservative Multimaterial Models

The present work is devoted to numerical approximation of multi-material flow governed by a genuinely non conservative hyperbolic system. We have to consider the surface tension force in a low Machregime. The propose strategy is based on an appropriated relaxed formulation of the Riemann problem and a dual time scale to properly filtered the acoustic. Numerical results are proposed for chock bubble interactions and the dynamic of a water drop falling under surface tension effects.

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MS90

Multi-Material, Incompressible Flow Simulations Using the Moment-of-Fluid (MOF) Method

We demonstrate second order accuracy in multi-material incompressible viscous flow simulations using the Moment-of-Fluid (MOF) method. The MOF method combined with a semi-Lagrangian material advection scheme demonstrates superior accuracy and reliability compared to traditional, first order accurate interface reconstruction schemes such as Youngs' method. The formulation and impact of different material properties, such as density and viscosity, and subcell averaging schemes in a volume tracking based simulation is also discussed.

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MS91

Separated Representations and Algorithms for Multidimensional Operators

Separated representation of multidimensional integral operators with radially symmetric kernels leads to fast algorithms for their application. This approach is also applicable to singular and hypersingular operators ubiquitous in physics. Such approximations and algorithms are already used in quantum chemistry and have a strong potential to address computational problems in other applications. The talk is an overview of the approach and some of its applications.

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MS91

Projection, Matching and Basis Pursuits for Multilinear Approximations

We discuss various greedy algorithms for best r-term approximations where the dictionary comprises a continuously varying family of elements. The context may be an approximation of tensors by a sum of decomposable tensors, of quantics by a sum of powers of linear forms, of operators by a sum of Kronecker products, or otherwise. The nearness measure could be a norm (that may not come from an inner product) or a non-metric distance like Bregman divergence.

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MS91

The Separated Representation of the Multiparticle Green's Function in Quantum Mechanics

The Green's function for an N-electron system in quantum mechanics is the inverse of a positive shift of the negative Laplacian, in 3N-dimensional space. It can be approximated by a sum of Gaussian convolutions, which are separable, and thus result in a separated representation that can be applied efficiently. We show that the number of Gaussians needed grows slowly in the allowed relative error in operator norm, and is independent of N and the shift.

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MS91

Approximation by Exponential Sums Revisited

In [Beylkin, Monzon: On approximation of functions by exponential sums. Appl. Comput. Harmon. Anal. 19-1 (2005)] we developed algorithms which can be used to approximate, for any given accuracy and with uniform error on any positive interval, a power function by a short exponential sum. An initial exponential sum approximation was derived from an integral discretization and we used the Euler-Maclaurin formula to estimate the sum length in terms of the accuracy and the interval size; a shorter approximation was obtained via a reduction algorithm. In this talk we present a different, simpler way to derive the initial approximation and estimate its length, and a more straightforward procedure to obtain the final, shorter sum approximation.

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MS92

On Numerical Properties of Ensemble Kalman Filter for Data Assimilation

Ensemble Kalman Filter (EnKF) has been widely used as a sequential data assimilation method, primarily due to its ease of implementation compared to the traditional Kalman filter. In this talk rigorous analysis on the numerical errors of the EnKF is conducted in a general setting. Error bounds are provided and convergence of the EnKF to the exact Kalman Filter is established. Numerical examples are provided to verify the theoretical findings and to demonstrate the performance of an efficient EnKF implementation.

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MS92

Effective Collocation Methods for Uncertainty

Quantification

Porous media in nature is highly heterogeneous and subject to uncertain due to the lack of sufficient data. Multiscale of uncertainty is present between and within the layers of porous media. A general framework that combines random domain decompositions (RDD) and probabilistic collocation method on sparse grids is proposed to resolve the large- and small-scales of uncertainty effectively. This combined approach is applied to the flow in porous media.

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MS92
Uncertainty Quantification in Chemical Systems

Uncertainty quantification (UQ) in chemical systems is significantly challenged by the non-linearity of chemical source terms. This non-linearity leads to fast rates of growth of uncertainty in the computed fields of species concentrations and thermodynamic variables. Capturing this rate of growth accurately and in a stable manner has placed constraints on the use of intrusive stochastic Galerkin methods for UQ using global polynomial chaos (PC) expansions, and has lead to the development of wavelet-based schemes with block decomposition of stochastic space. In this talk, we illustrate the use of wavelet-based PC UQ methods for ignition in chemical systems, with a specific focus on ignition with heat-release and associated growth of uncertainty.

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MS92
An Adaptive Hierarchical Sparse Grid Collocation Algorithm for the Solution of Stochastic Differential Equations

In recent years, there has been a growing interest in analyzing and quantifying the effects of random inputs in the solution of ordinary/partial differential equations. To this end, the spectral stochastic finite element method (SSFEM) is the most popular method due to its fast convergence rate. Recently, the stochastic sparse grid collocation method has emerged as an attractive alternative to SSFEM. It approximates the solution in the stochastic space using Lagrange polynomial interpolation. The collocation method requires only repetitive calls to an existing deterministic solver, similar to the Monte Carlo method. However, both the SSFEM and current sparse grid collocation methods utilize global polynomials in the stochastic space. Thus when there are steep gradients or finite discontinuities in the stochastic space, these methods converge very slowly or even fail to converge. In this work, we develop an adaptive sparse grid collocation strategy using piecewise multilinear hierarchical basis functions. Hierarchical surplus is used as an error indicator to automatically detect the discontinuity region in the stochastic space and adaptively refine the collocation points in this region. Numerical examples, especially for problems related to long-term integration and stochastic discontinuity, are presented. Comparisons with the multi-element generalized polynomial chaos and Monte-Carlo methods are also given to show the efficiency and accuracy of the proposed method.

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MS93
A Posteriori Error Estimates for Higher Order Elements

We describe a post processing derivative recovery scheme for the finite element solution u_h on general unstructured but shape regular triangulations. In the case of continuous piecewise polynomials of degree $p \geq 1$, by applying the global L^2 projection (Q_h) and a smoothing operator (S_h), the recovered p-th derivatives ($S_h^m Q_h \partial^p u_h$) superconverge to the exact derivatives ($\partial^p u$). Based on this technique we derive a local error indicator depending only on the geometry of corresponding element and the $(p+1)$-st derivatives approximated by $\partial S_h^m Q_h \partial^p u_h$. This is joint work with Jinchao Xu and Bin Zheng of Penn State.

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MS93
Flux Recovery and Accurate A Posteriori Error Estimators for Elliptic Problems

This talk will introduce two new estimators on finite element approximations to general elliptic problems. These estimators use recoveries of the flux in H(div) conforming finite element spaces. One of the estimators is exact in a norm on any given mesh without regularity assumptions. This means that the estimator is ideally perfect for error control on pre-asymptotic meshes, a paramount and difficult task in computation and that the estimator can be applied to non-smooth problems.

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MS93

An Efficient and Reliable Hierarchical Basis Error Estimate Requiring only H^1-regularity of the Exact Solution

For elliptic BVPs, the standard argument asserting the equivalence of a hierarchical basis error estimate with the actual error involves a strengthened-Cauchy inequality and a saturation assumption – the latter of these, although it generally holds asymptotically, depends strongly on things which are not readily measured. Without making use of any assumptions beyond H^1-regularity of the solution, we establish equivalence up to an additional, explicitly-computable data oscillation term.

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MS93

Flux Recovery Error Estimators for Second Order Elliptic Equations

We introduce new recovery-based a posteriori error estimators for diffusion equations. To overcome possible over-refinements of existing estimators of recovery type, we recover the flux in H(div)-conforming finite element spaces to accommodate possible discontinuities of the flux. The recovered flux is accurate in the L^2 norm for linear elements and in the H(div) norm for higher-order elements, respectively. The reliability and efficiency properties of the resulting estimators are established.

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MS94

Morphological Segmentation of Remote Sensing Images Based on Scale

In this work, we propose a segmentation method for remote sensing images based on scale profiles extracted by morphological analysis. More concretely, we use the topographic map, which represents an image by the hierarchical structure of its level lines, to extract the scale profile of a pixel. The scale profile is obtained by cumulating the contrast of the shapes (interior of connected components of level lines) containing this pixel. Based on the scale profiles extracted from the image, we associate a label to each pixel corresponding to the most significant shape containing this pixel. The main advantage of this approach compared to traditional morphological analyses is its auto-duality, that is, light and dark structures are treated equivalently. Experiments performed on real remote sensing images demonstrate the ability of the proposed approach to yield spatially accurate results.

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MS94

Variational Properties of a Segmentation Functional Depending on Curvature and with Linear Growth

A functional for image segmentation is considered wihich contains a bulk energy of the Mumford-Shah type and a geometric term depending on contour curvature. The geometric part of the energy includes the length of the curves of the segmentation, the number of their endpoints, and the integral of a function of curvature along the curves. The integral functional of curvature has linear growth at infinity with respect to the modulus of curvature as in the Nitzberg-Mumford segmentation model. As a consequence, the functional penalizes the amplitude of angles (changes of direction) at corner points and junctions which are not considered as endpoints of curves. A theorem of existence of minimizers is proved in a class of pairs (u, C) where C is a family of Sobolev curves having derivatives with bounded variation, and u is a Sobolev function outside of C. For any curve of the segmentation an argument function $\theta \in BV$ is defined which represents the angle (mod 2π) that the derivative of the curve forms with the direction of a fixed axis. Tangent vectors are identified with points of the unit circle S^1 and corners are considered in terms of jumps of the corresponding angles θ.

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MS94

Learning Sparse Dictionaries for Image Segmentation

In this talk I will present a new framework for image segmentation based on learned dictionaries. Classical methods perform the segmentation by finding homogeneous regions that do not deviate too much from a fixed pattern, for instance a gray level or a texture descriptor. Our framework enables non-linear deviations from the optimal model using a sparse expansion of the local image content on a set of optimized atoms. These set of atoms are packed into dictionaries adapted to each region of the segmentation. The segmentation problem is then expressed as a search for a set of dictionaries adapted to the sparse representation of local patches in the image. An iterative algorithm minimizes an energy that quantifies the sparsity of the patches inside each region of the segmentation. Numerical examples show the usefulness of this approach for the unsupervised segmentation of textured images. This is a joint work with Michael Elad and Nir Sochen.

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MS94

The Edge Strength Function: Harmonic Analysis

Perspective

The edge strength function is the minimizer of the Ambrosio-Tortorelli approximation of the Mumford-Shah functional. In its original form, it is presented as an aid in local symmetry computation (Tari and Shah 98). In this talk, I will relate the edge strength function to harmonic analysis in the sense of global expansions in special functions that are related to spectrums of certain differential operators. This insight opens up new possibilities in shape representation and segmentation. In particular, I will focus on how features (of varying locality) are captured by global expansions.

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MS95
Building a Successful, Scalable Parallel Numerical Library: Lessons from PETSc

The PETSc library is widely used for the solution of partial differential equations on parallel computers. This talk discusses some of the reasons for the success of PETSc. These include the use of mathematical concepts, rather than a design based on particular algorithmic choices, to organize the library and to effectively hide the details of the parallel implementation from the user. Other issues include completeness of operation and clean interfaces to allow extensions to new algorithms and interactions with other numerical libraries.

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MS95
The Role of Compilers in Managing Application and Architecture Complexity

Modern computer architectures are undergoing a paradigm shift, where every microprocessor, from embedded to desktop to supercomputing socket, will be a parallel architecture. Alongside increased application complexity, this trend poses enormous challenges for application developers in obtaining acceptable performance. We discuss the role of compiler technology in managing this complexity by exploiting performance-enhancing features offered by target architectures while freeing programmers from low-level details. We describe a systematic approach to performance tuning of key computations.

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MS95
Building Symbiotic Relationships Between Formal Verification and High Performance Computing

Computational simulation for scientific and engineering applications are becoming more ubiquitous as part of the engineering design cycle. The application of simulation science to complex problems often requires complex models, sophisticated numerics and intricate implementations. Tremendous effort has been expended toward the development of systematic techniques for model validation and numerical method verification. As most researcher's hesitantly admit, the amount of time spent debugging intricate high performance parallel implementations of their simulations consume a large bulk of their time. In particular, many would argue that although this debugging time is necessarily, it distracts one from the science or engineering problem of interest. In this talk, we will present our continuing effort by the Utah Gauss Group to employ formal verification techniques to the debugging of parallel high performance computing codes using MPI. This synergistic combination of formal techniques with HPC is designed to infuse news ways of thinking about parallel code design through interaction of two normally disparate communities, with the goal of benefiting both communities.

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MS95
Automated Dynamic Test Generation for Software Systems

Testing with manually generated test cases is the primary technique used in industry to improve reliability of software–in fact, such testing is reported to account for over half of the typical cost of software development. I will describe Concolic Testing, a systematic and efficient method which combines random and symbolic testing. Concolic testing enables automatic and systematic testing of large programs, avoids redundant test cases and does not generate false warnings. Experiments on real-world software show that concolic testing can be used to effectively catch various generic errors.

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MS96
A Multi-Scale Model of Large Scale Tropical Flows

The IPESD multi-scale asymptotic framework of Majda and Klein has proved to be enormously successful in simplifying the equatorial primitive equations to yield self-consistent multiscale models. Among these is the synoptic/planetary scale MJO model of Biello and Majda. In this talk we will describe a generalization of this multi-scale framework which we call the Moist Synoptic Planetary Intraseasonal Equatorial Dynamics equations (M-SPIED) and show how the three cloud-type model of Khouider and Majda can be incorporated into this asymptotic framework. We will describe a fully non-linear and multiscale MJO model with upscale fluxes from sypnoptic to planetary scales and feedback to the synoptic scale from mean flows on the planetary. In order to balance the various terms in the asymptotics, we will find that a stronger, large scale zonal wind must be included in the derivation. Considering this flow in conjunction with the lowest order meridional circulation, we find that this corresponds exactly to the Hadley circulation and the Trade Winds. The ultimate result is the first self-consistent, multi-scale MJO model interacting with the Hadley circulation, both of which are driven by heat and moisture fluxes from the synoptic scales.

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MS96

Moist Frontogenesis in Axisymmetric Hadley Circulations

A previous theory of eyewall formation in tropical cyclones is adapted to axisymmetric Hadley circulations to show that both wind-induced surface heat exchange (WISHE) and the horizontal advection of subcloud entropy exert frontogenetic tendencies on the intertropical convergence zone. In particular, WISHE shifts the subcloud entropy peak toward the equator, thereby reducing the critical forcing needed to produce angular momentum conserving Hadley flow. The relevance of these results to the onset of monsoons is discussed.

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MS96

Interactions Between the MJO, Convectively Coupled Kelvin Waves, and Mid-latitude Flow

Convection within the active convective phase of the MJO is largely concentrated within synoptic scale waves. Convectively coupled Kelvin waves frequently move eastward together with and at similar phase speeds to synoptic scale mid latitude waves. This presentation will demonstrate systematic amplification of these mid latitude waves in response to Kelvin wave convection within the active phase of the MJO.

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MS96

Convectively Coupled Gravity Waves in the Tropics

Tropical deep convection has long been known to interact strongly with large-scale atmospheric wave circulations – well known examples include convectively coupled Kelvin waves and the Madden-Julian Oscillation, both of which have characteristic spatial scales measured in 1000s of kilometers. In addition to these synoptic scale waves, however, we present evidence for zonally-propagating inertio-gravity gravity wave disturbances with spatial scales typically on the order of 100s of kilometers and frequencies ¡ 2.5 day. These short/fast waves are shown to be strongly tied to the diurnal cycle over land, and to appear prominently near certain geographic features, such as the eastern mountains of Rwanda, the central mountains of New Guinea, and the northeastern coast of Brazil. We also provide evidence that some of these disturbances may be involved in the genesis of tropical storms, such as Hurricane Andrew 1992.

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MS97

Sparse Collocation Method for Stochastic Fredholm Equations of Second Kind

We develop the fast collocation methods for the second kind integral equations with stochastic loading resulted from PDEs with random boundary condition. The well-posedness of the discretization scheme is proved. The sparse-grid multi-scale bases are constructed, associated with which a truncation strategy is proposed so that the computational complexity is reduced to be linear up to a logarithmic factor. The convergence rate is not ruined by the truncations.

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MS97

Non-Traditional Stochastic Partial Differential Equations

A solution of a traditional stochastic evolution equation is a square-integrable adapted process. By defining the solution using a chaos expansion, we relax the integrability and adaptedness requirements and greatly enlarge the class of equations admitting a solution, to include, in particular, bi-linear stochastic elliptic equations and bi-linear stochastic parabolic equations with second-order derivatives in both drift and diffusion parts. The same tools of chaos expansion also allow us to consider stochastic perturbations other than the standard Brownian motion, including (but not limited to) the fractional Brownian motion.

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MS97

Efficient Collocational Methods for Stochastic Computations

Collocation methods have become popular in recent years and are widely used in stochastic computations. In this talk we review the framework of stochastic collocation methods and their efficient implementations. Attention will be paid to problems with high dimensionality, i.e., those involving large number of random variables.

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MS97

A Non-Linear Dimension Reduction Methodology for Generating Data-Driven Stochastic Input Models

Stochastic analysis of random heterogeneous media provides information of significance only if realistic input models of the topology and material property variations are used. This work introduces a framework to construct such input stochastic models for the topology, thermal diffusivity and permeability variations in heterogeneous media using a data-driven strategy. Given a set of microstructure realizations (input samples) generated from given statistical information about the medium topology, the framework constructs a reduced-order stochastic representation of the topology and material properties. This problem of constructing a low-dimensional stochastic representation of property variations is analogous to the problem of manifold learning and parametric fitting of hyper-surfaces encountered in image processing and psychology. Denote by M the set of microstructures that satisfy the given experimental statistics. A non-linear dimension reduction strategy is utilized to map M to a low-dimensional region, A. We first show that M is a compact manifold embedded in a high-dimensional input space R^n. An isometric mapping F from M to a low-dimensional, compact, connected set $A \subset R^d$, $d < n$, is constructed. Given only a finite set of samples of the data, the methodology uses arguments from graph theory and differential geometry to construct the isometric transformation $F : M \mapsto A$. Asymptotic convergence of the representation of M by A is shown. This mapping F serves as an accurate, low-dimensional, data-driven representation of the property variations. The reduced-order model of the material topology and property variations is subsequently used as an input in the solution of stochastic PDEs with multiscale futures that describe the evolution of the dependent variables. A sparse grid collocation strategy (Smolyak algorithm) with piecewise multi-linear hierarchical interpolation functions is utilized to solve these stochastic equations efficiently. We showcase the methodology by constructing low-dimensional input stochastic models to represent thermal diffusivity and permeability in porous media. These models are then used in analyzing the effects of topological variations on the evolution of temperature and flow in random heterogeneous media.

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MS98

Effects of Director Angle Anchoring Conditions on the Dynamic Moduli of Heterogeneous Nematic Polymers

We examine the influence of director angle anchoring conditions on the linear viscoelastic response of heterogeneous nematic polymers to small amplitude oscillatory shear flow. First, for normal and tangential anchoring, we recover explicitly solvable Leslie-Ericksen behavior and observe significant anchoring effects. Then, numerical studies of the more complicated system with anchoring conditions near 45 degrees show significantly different high-frequency scaling for the storage modulus.

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MS98

New Phases in Biaxial LCPs

In 2004, a new "biaxial phase" of liquid crystalline polymers was discovered experimentally. Since then, a lot of effort has been devoted at the experimental level to understand the orientational response of such a system in the presence of an external field. It was quickly realized that the response of such an elusive system is difficult to predict experimentally and require extreme conditions of temperature, pressure and high electric/magnetic fields. To our knowledge, for the first time, we predict and present the various phases of biaxial LCPs and show the sequence of orientations in the material parameter region. The underlying hydrodynamic theory; as well as; the rheological properties are also discussed.

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MS98

General Kinematic Transport in Liquid Crystal Dynamics

Ericksen Leslie model is widely accepted in the study of nematic liquid crystal materials. In this talk, we will present some existence results for the system with general transport equation for the orientational field. Such transport relation reflect the microscopic properties such as the shape of the molecules, slippery boundary conditions, molecular packing, etc. They bring extra difficulties in the study of the well-posedness of the system, especially the lose of the maximal principle in the direction field.

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MS98

Rheological Properties of Biaxial Liquid Crystal Polymers

In this talk, we will report some latest results on rheological properties of biaxial liquid crystal polymers under shear. These results are obtained by solving the Smoluckowsi equation for biaxial liquid crystals using a Garlerkin method employing the Wigner function expansion of the probability function. Various novel phases under shear will be exhibited and their rheological consequence reported.

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MS99

Automated Tracking for Alignment of Electron Microscope Images

We present a method for automatic full-precision alignment of the images in a tomographic tilt series. Full-precision automatic alignment of electron microscopy images has remained a difficult challenge due to the limited electron dose and low image contrast. We frame the problem probabilistically as finding the most likely particle tracks given a set of noisy images, using contextual information to make the solution more robust to the noise in each image. To solve this maximum likelihood problem, we use Markov Random Fields (MRF) to establish the correspondence of features in alignment and robust optimization for projection model estimation.

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MS99

Advances in Electron Microscope Instrumentation and Exploration of Biological Structures

As we accrue massive amounts of data on gene sequences and protein structure, we must integrate this data into more elaborate models. The cellular ultrastructure which provides substrates whereby molecules are organized and cellular processes are constrained. To address the problem of understanding biological structure, we have expanded several technologies around the electron microscope to include both high-resolution light microscopes and high voltage electron microscopes. We have developed new imaging modes and instrument designs, to increase the spatial range and resolution of imaging. Our work on image processing and computer graphics includes 2-4D imaging for both light and electron microscopy.

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MS99

Mathematics of Electron Microscope Tomography

In the first part (Lawrence) we summarize work on an EM tomography package, TxBR, and mathematical problems associated with alignment and reconstruction. The techniques include projective duality and nonlinear bundle adjustment; Fourier integral operators and ultrahyperbolic equations. In the second part (Cunha) we describe recent work in denoising cryoimages for EM tomography using nonlinear unsupervised filtering. We borrow ideas from the nonlocal means method and introduce a L1 metric to assess similarity between neighboring regions to offer a robust filter at a reduced cost.

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MS99

Local Tomography in Electron Microscopy

Tomographic techniques, in which samples are viewed from multiple directions, are used in electron microscopy. Often, the molecules are all different (rather than copies of one single molecule in different orientations), and one wants to image the individual molecules. Therefore, any algorithm for this problem must reconstruct each molecule independently. The problem is local because the electron beam is only wide enough to penetrate a small part of the object. Furthermore, the data are limited angle since the object cannot be rotated through a full 180 degrees. For these reasons, some data are missing, and inversion is unstable. The author will use microlocal analysis to explain this instability, and he will present a refined local algorithm and reconstructions (pictures) using his algorithm.

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MS100

Interface Reconstruction and Sub-Zone Physics Models

We present our recent work on interface reconstruction in a logically structured Lagrangian CFD code that now incorporates the MoF system developed by Shashkovs group at LANL. We also discuss the models used to update the state variables in the mixed cells during the Lagrange step, and the methods used for remapping the state variables after an ALE step. LLNL-ABS-401564

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MS100

A Fast Geometric Mesh Untangling Algorithm for ALE Methods

The rezone step in an ALE method relies on mesh smoothing that is perhaps triggered by some mesh quality indicators to keep the computational mesh valid. We have developed a 2D robust mesh untangling algorithm that is purely geometric and does not rely in numerical optimization. This algorithm builds on the feasible set untangling method and our novel weak untangling approach that can be viewed as a discrete efficient version minimization based untangling method.

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MS100

Dynamic Volume Fraction Evolution in Multipressure Multiphase Flow Models

Multpressure multiphase flow models require additional closure relations to determine the individual pressures of the different phases. These relations often take the form of volume fraction evolution. We present a rigorous theoretical framework for constructing such equations in terms of submodels for the relative expansion rates of the phases. We also present a simple provisional submodel in which the phases dynamically expand or contract in response to pressure differences, and relax toward local pressure equilibrium.

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MS101

Computational Analysis of Dynamic Social Networks

Recent technologies are producing a wealth of very detailed data about social behavior in human and animal populations. Yet traditional social network analysis aggregates interactions over time and the information on the order and timing of events is discarded. We present a computational framework for analysis of explicitly dynamic social networks. We have developed techniques for identifying persistent dynamic communities, influential individuals, and extracting interaction patterns. We demonstrate our approach by analyzing interactions among zebra populations.

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MS101

Reverse Engineering of Networks Via the Modular Response Analysis Method

The reverse engineering problem is, loosely speaking, that of unraveling the web of interactions among the components of protein and genetic regulatory networks. A major goal is to map out the direct functional interactions among components, a problem that is difficult to approach by means of standard statistical and machine learning approaches such as clustering into co-expression patterns. Information on direct functional interactions throws light upon the possible mechanisms and architecture underlying the observed behavior of complex molecular networks. An intrinsic difficulty in capturing such interactions in intact cells by traditional genetic experiments, RNA interference, hormones, growth factors, or pharmacological interventions, is that any perturbation to a particular gene or signaling component may rapidly propagate throughout the network, thus causing global changes which cannot be easily distinguished from direct (local) effects. Thus, a central goal is to use the observed global responses (such as steady-state changes in concentrations of activated activities of proteins, mRNA levels, or transcription rates) in order to infer the local interactions between individual nodes. One potentially very powerful approach to solve the global to local problem is the Modular Response Analysis (MRA) method. We first describe the MRA method, and then we formulate an experimental design problem that arises when using the approach. For large networks, this problem will not scale well, and is computationally hard. This suggests an interesting computational complexity theoretical problem, closely related to set cover questions. We provide an efficient approximate solution algorithm for this computational problem.

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MS101

Why Do Hubs in the Yeast Protein Interaction Network Tend to be Essential: Re-Examining the Connection Between the Network Topology and Essentiality

The fact that high-degree nodes in a protein interaction network tend to correspond to proteins that are essential, suggests that the topological prominence of a protein in a protein interaction network may be a good predictor of its biological importance. Several hypotheses about putative connections between essentiality of hubs and the topology of protein-protein interaction network have been proposed, but as we demonstrate, these explanations are not supported by the properties of protein interaction networks. We propose an alternative explanation.

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MS101
Defining, Inferring, and Encoding Modularity

Over the last decade, one of the driving problems in systems biology has been to find "modules" in biological networks. A bewildering variety of definitions of modules have ensued, along with a corresponding multitude of methods for finding these modules and quantifying the modularity of either a biological network or of a particular partitioning of a network. In this talk I'll discuss how two very old ideas — statistical inference and rate-distortion theory — can be used to infer modules (along with inferring the true number of modules in a network) and to reveal the modules as an optimal encoding (suggesting an order parameter for modularity which makes reference to no fixed partition or scale). I hope also to illustrate how this driving systems biology problem relates to an older literature in "community detection" (from the social sciences) and "graph partitioning" (from computer science and discrete mathematics).

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MS102
On Multi-Variable Representations with Sums of Exponentials

An efficient representation of multi-variable functions via (a separable) sums of exponentials has many applications in numerical analysis and signal processing. Obtained for a finite but arbitrary accuracy in the case of single variable, such representations typically have significantly fewer terms than corresponding Fourier expansions. We present examples of these approximations, discuss their applications and describe current work towards multidimensional extensions of our approach.

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MS102
Low Rank Approximations of Matrices and Tensors

In many applications, it is of interest to approximate data, given by m by n matrix A, by a matrix B of at most rank k, which is much smaller than m and n. The best approximation is given by singular value decomposition, which is too time consuming for very large m and n. We present here an optimal least squares algorithm for computing a k-rank approximation to the data consisting of m by n matrix A by reading a number of rows and columns of A. This algorithm can be applied to nonnegative matrices and to tensors.

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MS102
The Polar Curvature Tensor and Hybrid Flat-surfaces Modeling

The polar curvature describes the d-dimensional flatness of $d + 2$ points in a Euclidean space. We utilize the polar curvature tensor to form a multi-way spectral clustering algorithm for solving the problem of segmenting data sampled from a mixture of sufficiently flat surfaces. Using tensorial algebra and matrix perturbation theory, we prove that, with high probability, our proposed algorithm segments the different underlying surfaces well. We exemplify application of the algorithm to several real-world problems.

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MS102
On a Generalisation of Sylvester Method for Symmetric Tensor Decomposition

In 1886, J.J. Sylvester proposed a method to decompose a binary form into a minimal sum of powers of linear forms, based on rank and kernel computation of specific Hankel matrices. In this talk, we will revisit this approach for multivariate polynomials from a dual point of view, show how it is related to normal form computation and to truncated moment problems and describe an algorithm to compute such a decomposition.

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MS103
High-Resolution, Two-Phase Flow Modeling Challenges for Light Water Nuclear Reactors

It readily apparent that a resurgence of nuclear power in the U.S. will very likely involve a newer generation of light water reactors (LWRs). Within the context of multiphase flow situations that can occur in either normal or off-normal operation of light water nuclear reactors, this presentation will address the need to simultaneously solve fluid dynamic interface problems as well as multiphase mixtures arising from boiling, cavitation, and bubble collapse in both high- and low-speed flow conditions. It will present the multi-scale challenges of providing highly resolved details where necessary, simultaneously with large scale system simulation. The need for well-posed models will be emphasized as will the need for well-balanced spatial and temporal discretization. Important side-bar issues of compressibility and need for conservative-form equation systems will be discussed.

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MS103

Mesh Adaptivity and A Posteriori Error Estimation for HiFi Simulations in Nuclear Science and Engineering

We will present advances in mesh adaptivity based on a posteriori error estimators for various multigroup neutron balance equations: from diffusion and simplified PN equations to discrete ordinates SN equations. In doing so, we will review error estimators used for elliptic (diffusion) and hyperbolic (transport) systems. Balance equations present some specific challenges for mesh adaptivity and require special attention: coupling between energy groups, angular moments or angular directions. Numerical validation will be presented.

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MS103

Foundational Development of a Next Generation Nuclear Reactor Safety Code

A multi-scale modeling and simulation strategy for addressing coupled physics (e.g. heat transfer, turbulent flow, neutronics, thermal mechanics) at the fuel-pin (mm), in-vessel component (cm-m), and reactor system (1-30 m) scales in complex geometries is described. A multiphysics solver written in python is used to drive a spectrum of coupling algorithms ranging from traditional weak coupling based on successive substitution, to strong coupling based on various implementations of Jacobian-Free Newton-Krylov (JFNK).

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MS103

Real World Application of Nonlinear Acceleration Methods in Light Water Reactor Analysis

Existing applications of non-linear acceleration methods in modern LWR core neutronic analysis will be reviewed. These methods include a class of techniques used to make possible the practical solution of large-scale, 3-D, multigroup, neutron transport and diffusion eigenvalue problems. Ideas for extending such methods to the acceleration of Monte Carlo neutron transport problems will also be presented.

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MS104

Pointwise A Posteriori Error Estimation for Parabolic Problems

A posteriori estimation of pointwise errors is often physically interesting but technically challenging. In this talk we describe how the *elliptic reconstruction* technique introduced by Makridakis and Nochetto can be employed to obtain a posteriori estimates in the maximum norm for a backward Euler/finite element discretization of the heat equation on arbitrary (nonconvex) polyhedral domains.

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MS104

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

Significant problems face the use of adaptive discretization for evolution problems, including global error control of quantities of interest, accounting for cancellation of error and changing stability, and dealing with the affects of mesh refinement on accuracy and stability. We describe recent work addressing these issues, including a probabilistic framework replacing the standard optimization framework, a blockwise-adaptive parallel-efficient adaptive strategy, and the use of coarse scale adjoint information for error estimation.

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MS104

An *A Posteriori* Error Estimator For A Quadratic C^0 Interior Penalty Method For The Biharmonic Problem

In this talk we present a reliable and efficient residual-based *a posteriori* error estimator for a quadratic C^0 interior penalty method for the biharmonic problem on polygonal domains. We will outline the *a posteriori* error analysis, which involves new tools that can be applied to other finite element methods for fourth order problems, and also present numerical results that illustrate the performance of the error estimator. This is joint work with Susanne C. Brenner and Li-yeng Sung.

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MS105

Optimal Unstructured Meshes and Spectral Conditioning Estimates for FEM

We discuss optimal unstructured simplicial meshes (in particular three dimensional tetrahedral meshes) for the numerical solutions of PDES based on the CVT technology. We also illustrate in precise terms how they affect the spectral conditioning of the linear algebraic systems resulted from general finite element discretizations.

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MS105

The Role of Centroidal Voronoi Diagrams in Phyllotaxis

Phyllotaxis study the arrangement of repeated units such as leaves, steams, seeds in plants. The most commonly known are spiral patterns found in plants, such as the arrangement of seeds in the sunflower or the pineapple. Very often regular patterns are found, in which the numbers of right- and left-turning spirals respectively are given by two successive Fibonacci numbers. Pursuant to the classical theory this results from the fact that the divergence angle, i.e. the angle between two successive features, is near the Golden angle. The central question of phyllotaxis is: why are these characteristic patterns so common in the empire of plants? For the description and analysing of such patterns often Voronoi-regions were used. As an example, in 1948 Richards constructed a Voronoi tesselation for a set of points which were placed using the Golden Angle to visualize their uniform placement on a disc. In recent works we presented a simple, biologically motivated contact pressure model for the creation of phyllotactic patterns and their computer simulation. We compute the contact pressure between botanical units on the basis of local centroidal Voronoi relaxation. Using this method in combination with Hofmeisters rule for placing new units creates stable patterns with high-order Fibonacci spirals for a large range of initial conditions.

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MS105

Nondegeneracy and Weak Global Convergence of Lloyd Algorithm

Lloyd iteration is currently the most popular and elegant algorithm for computing centroidal Voronoi tessellations and optimal quantizers, but many questions remain about its convergence, especially in d-dimensional spaces with $d > 1$. In this talk, we present some recent progresses on the convergence of Lloyd algorithm. We show that any limit point of the Lloyd iteration in any dimensional spaces is non-degenerate provided that the domain is a convex and bounded set, and the density function belongs to L^1 and is positive almost everywhere. This assures that the fixed point map remains closed and hence the standard theory of descent methods guarantees weak global convergence of the Lloyd iteration to the set of non-degenerate fixed-point quantizers.

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MS105

Binning the Cosmos: Astrophysical Applications of Voronoi Tessellations

Certain astrophysical phenomena, ranging in size from the granulation patterns on the surface of the Sun to the large-scale distribution of galaxies in the cosmos, give a strong visual impression of being geometrically related to Voronoi tessellations (VTs). In the cosmological context, opinions have differed as to whether this resemblance points to a fundamental physical process that produces actual VTs in nature, or merely suggests that VTs are useful statistical tools to describe the distribution of galaxies or to simulate them as a testbed for other techniques. In the past decade, evidence has accumulated that physical models producing natural VTs are not consistent with other cosmological observations, most notably the temperature fluctuations in the cosmic microwave background radiation. Nonetheless, VTs continue to be used by astronomers in a several important applications, including: (1) detecting astronomical sources in high-energy observations, where the number of detected photons is small; (2) identifying clusters of galaxies in the sparsely populated universe; (3) adaptive binning of data in situations where a uniform signal-to-noise ratio is required and/or the data are sparse, to produce geometrically unbiased maps; and (4) as a tool in particle-based simulations to set up initial conditions without imposing a regular grid. This talk will review some of the history of VTs in extragalactic astronomy and cosmology, describe the current state of the art in their application, and suggest some future applications and algorithmic needs.

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MS106

From Matrix Laboratory to Technical Computing Environment - Growth of MATLAB(R) and The MathWorks(TM)

MATLAB(R) started in the late 1970s as an academic package for matrix computations and has grown into a mature technical computing environment with a rich layer of additional products and interaction with other languages and environments. The MathWorks(TM) has grown from a tiny startup into an international company. Come hear how we faced the technical, operational and organizational challenges as we grew from academic tool to industrial strength scientific computing software.

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MS106

Sparse Matrix Research and Software Development at the University of Florida

The speaker has a long history of writing software for academia, industry, and government. Why should an academic write good code? It's a multi-constraint challenge. To publish, the code must reflect new research ideas; most academics stop there, although publishing code in ACM TOMS can help. For academics, writing robust code is not unlike writing a sorely-needed textbook, with an impact that can exceed most journal articles. Royalty, consulting, and licensing issues are also discussed.

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MS106

A Software Lifecycle Model for Research to Production Software

A research based software project is complex and multistage. We are tasked to develop algorithms and software that are leading-edge, to solve previously intractable problems. Eventually, we must deliver robust and hardened software. We present a three-phase promotional lifecycle model that closely matches the needs and realities of many developers. Small algorithms-focused efforts can develop in a dynamic, customer-interactive environment while mature projects can drive toward a fully-certified software environment necessary for production computing.

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MS106

Software Engineering Challenges in the Development of a Commercial CFD Application

FLUENT is a commercial Computational Fluid Dynamics package for engineering simulation and analysis. It is capable of simulating applications that include turbulent fluid flow and heat transfer, multiphase, and reacting flow, on stationary and moving/deforming meshes. Industrial problems often require the solution of discretized equations with excess of a billion unknowns, necessitating the use of contemporary parallel computers. We will discuss lessons learned in its development, with emphasis on supporting diverse and evolving computing infrastructures.

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MS107

Slow Manifolds, Canards and Mixed-Mode Oscillations Near a Folded Node

We investigate the geometry of two-dimensional slow manifolds and the organization of associated canard solutions in the normal form of a folded node of a slow-fast vector field in $\mathbf{R}^3$. Furthermore, we demonstrate how a folded node gives rise to mixed-mode oscillations in the self-coupled FitzHugh–Nagumo system.

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MS107

A Boundary Value Problem Approach to Invariant Manifolds in Slow-Fast Systems

Systems with multiple time scales may display special types of solutions, including canard orbits and mixed-mode oscillations, where sections of the trajectory follow unstable slow manifolds. Finding the underlying invariant manifolds is a challenge in light of the extreme sensitivity of the initial value problem in this class of systems. We discuss a general boundary value problem formulation and demonstrate how it can be used for the reliable computation of two-dimensional invariant manifolds and canards in systems with two slow and one fast variable.

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MS107

Numerical Computation of Isochrons

For a dynamical system with a stable periodic orbit, an isochron is a set of initial conditions resulting in oscillations having the same phase. Different numerical techniques for calculating isochrons will be presented. For planar fast-slow dynamical systems, it is found that isochrons can accumulate very close to an unstable slow manifold, which presents a challenge for their numerical computation. Such accumulation has important implications for phase resetting under appropriate large perturbations.

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MS107

Mixed-Mode Dynamics and the Canard Phenomenon: Towards a Classification

Mixed-mode dynamics is complex dynamical behavior that is characterized by an alternation of small-amplitude (subthreshold) oscillations and large (relaxation-type) excursions. Using geometric singular perturbation theory and desingularization (blow-up), we propose a unified approach for studying this dynamics in the context of three-dimensional multiple-time-scale systems. We show that the mixed-mode behavior in such systems is due to an underlying canard phenomenon, and we indicate how the structure of the resulting mixed-mode oscillations can be classified accordingly.

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MS108

Improving Robustness of Algebraic Multigrid

One of the ingredients contributing to the success of algebraic multilevel methods based on smoothed aggregation is their ability to capture the near-nullspace of the solved problem on all levels of the multigrid hierarchy. For many problems, the critical near-nullspace components are not a priori known. The recently developed adaptive smoothed aggregation method was designed to alleviate such situations. We will describe the adaptive smoothed aggregation and discuss the latest developments in the method. Numerical examples will be presented demonstrating efficacy of the approach.

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MS108

Modern and Classical Theory for Adaptive Algebraic Multigrid

In recent years, substantial effort has been focused on the development of robust multigrid techniques for the solution of linear systems that are not efficiently treated by classical preconditioners. These adaptive multigrid methods were first motivated heuristically, based on the weak approximation properties that arise in classical algebraic multigrid theory. In this talk, I will discuss recent efforts to directly apply both classical and more recent algebraic theory for multigrid methods to these algorithms.

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MS108

Adaptive Algebraic Smoothers

This talk will present a new method of adaptively constructing smoothers based on Local Sensitivity Analysis (LSA). Given a linear system, Ax=b, LSA identifies blocks of the matrix, A, so that a smoother, such as block iterative Gauss-Seidel, can be constructed based on the identified blocks. Results will be presented for constant and variable coefficient elliptic problems, systems arising from scalar and coupled system PDEs, as well as linear systems not arising from PDEs.

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MS108

Incorporating Eigensolvers into the Current Adaptive Smooth Aggregation Framework

Consider the linear system $A\mathbf{x} = \mathbf{b}$, where A is a large, sparse, real, symmetric, and positive definite matrix and $\mathbf{b}$ is a known vector. Solving this system for unknown vector $\mathbf{x}$ using a smoothed aggregation multigrid (SA) algorithm requires a characterization of the algebraically smooth error, meaning error that is poorly attenuated by the algorithm's relaxation process. For many common relaxation processes, algebraically smooth error corresponds to the near-nullspace of A. Therefore, having a good approximation to a minimal eigenvector, or an eigenvector that corresponds to the minimal eigenvalue of A, is useful to characterize the algebraically smooth error when forming a linear SA solver. We discuss the details of a generalized eigensolver based on smoothed aggregation (GES-SA) that is designed to produce an approximation to a minimal eigenvector of A. We propose how GES-SA would be used with the current adaptive SA framework, and make comparisons with the current relaxation-based approach to investigate how eigensolvers may be employed for a possibly more efficient and robust adaptive method.

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MS109

Ensemble Level Multiscale Finite Element Methods

In this talk, we propose a stochastic mixed multiscale finite element method. The proposed method solves the stochastic porous media flow equation on the coarse grid using a set of pre-computed basis functions. The pre-computed basis functions are constructed based on selected realizations of the stochastic permeability field, and furthermore the solution is projected onto the finite dimensional space spanned by these basis functions. We employ multiscale methods using limited global information since the permeability fields do not have apparent scale separation. The proposed approach does not require any interpolation in stochastic space, and can easily be coupled with interpolation based approaches to predict the solution on the coarse grid. Numerical results are presented for permeability fields with Gaussian and exponential variograms.

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MS109

Nonparametric Density Estimation for Elliptic Problems with Random Perturbations

We describe an efficient numerical method for nonparametric density estimation for quantities of interest computed from an elliptic problem with randomly perturbed parameters and data. The method employs the finite element method, non-overlapping domain decomposition, and the Neumann series for an invertible operator. We use an a posteriori error estimate using adjoint operators and variational analysis to distribute computational work in order to achieve a desired accuracy by an efficient distribution of computational resources.

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MS109

Dynamic Data Driven Simulation in Stochastic Environment

To improve the predictions in dynamic data driven simulations (DDDAS) for subsurface problems, we propose the permeability update based on observed measurements. Based on measurement errors and a priori information about the permeability field, such as covariance of permeability field and its values at the measurement locations, the permeability field is sampled. This sampling problem is highly nonlinear and Markov chain Monte Carlo (MCMC) method is used. We show that using the sampled realizations of the permeability field, the predictions can be significantly improved and the uncertainties can be assessed for this highly nonlinear problem.

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MS109

Moment Statistics for Flow and Transport in Randomly Stratified Media

Parameters of geophysical systems are usually uncertain, so they are often represented as random fields. Parametric uncertainty can be propagated to the dependent variables of geophysical systems through stochastic pdes. Solutions of such pdes are complicated by the nonstationarity of the underlying parameters. I will discuss models of flow and transport through geophysical media that address nonstationarity in the stratified media that are found in many domains of geophysics including groundwater and atmospheric science.

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MS110

Using Sieve for Particle Tracking, Embedded Meshing and Field-Particle Interaction Computations

We have developed a powerful abstract formalism, called Sieve, for handing of distributed meshes and other geometric data. In this talk we will describes Sieve's capabilities for handing embedded meshes and tracking of particles and filaments interacting with the ambient medium. The applications include interactions of filaments with a visco-elastic matrix and electrostatic interactions of charge particles in a dielectric medium.

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MS110

Combinatorial Dataflow Analysis for Differentiation of High-Level PDE Representations

Efficient algorithms for large-scale PDE-constrained optimization, uncertainty quantification, and physics-based preconditioning require the creation of discrete operators not commonly available from simulation codes. In this talk we describe the underlying mathematical algorithms behind a software system for efficient in-place Frechet differentiation of symbolic problem representations for use in discretization of weak equations and their derivatives. In particular we focus on a combinatorial data flow analysis through which sparse evaluation is maintained.

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MS110

Exploitation of Jacobian Scarcity

We describe efforts within the automatic differentiation tool OpenAD to transform the computational graph of the function F into an equivalent graph that possesses as few nontrivial edges as possible. The goal is to exploit Jacobian scarcity, which can be seen as a generalization of other notions such as sparsity and rank deficiency. We present heuristics that have achieved an improvement factor of up to three in experiments.

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MS110

Hypergraph-Based Combinatorial Optimization of Matrix-Vector Multiplication

Kirby, et al. showed that combinatorial optimization of matrix-vector multiplication can lead to faster evaluation of finite element stiffness matrices. Based on a graph model characterizing row relationships, an efficient set of operations can be generated to perform matrix-vector multiplication. We improve the graph model by extending the set of binary row relationships, yielding significantly improved results over previous graph models. We also extend the representation by using hypergraphs to model more complicated row relationships and further improve the results.

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MS111

A New Class of Physics-based Solvers for Multiphase-Flow

We introduced a new class of physics-based preconditioners that exploits the porous media connectivity described by rock properties. The topology of this connectivity is computed with the aid of highly efficient percolation algorithms. Thus, transmissibility coefficients can be separated in several blocks corresponding to different percolative clusters and further reduced via deflation or agglomeration. The proposed class of preconditioners seems to be promising for solving a wide range problems arising from complex multiphase scenarios.

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MS111

Progress and Challenges using PETSc Algebraic Solvers in the PFLOTRAN Subsurface Reactive

Flow Code

We describe our experiences developing PFLOTRAN, a code for the fully implicit simulation of coupled thermal-hydrologic-chemical processes in variably saturated, non-isothermal, porous media. Our eventual goal is to conduct simulations involving 10-20 billion degrees of freedom; this presents considerable challenges for the underlying solvers provided by the PETSc framework. We outline the difficulties encountered and progress made as we have worked towards this goal on Jaguar, the Cray XT4 system at Oak Ridge National Laboratory.

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MS111

Modeling and Simulation of Non-Darcy Single-phase Flow through Heterogeneous Porous Media

An advection-reaction system of partial differential equations (PDEs) is proposed to model 2D single-phase flow in the non-Darcy regime. Sundance, a finite element PDE simulation framework from Sandia National Laboratories, is used to solve the system in parallel. Parallel implementation is necessary to fully resolve the block heterogeneity of the porous medium. Results will focus on solver techniques as well as the relationship between the porous medium heterogeneity and the advection terms in the model.

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MS111

Multi-Stage Preconditioning for Coupled Unstructured Reservoir Models and Multi-Segment Wells

A two-stage CPR (Constrained Pressure Residual) method is used to solve the linear systems of coupled reservoir models and multi-segment wells. An algebraic reduction of the coupled system is used, in which the multi-segment wells are reduced to their equiavalent “standard” well representation. Algebraic multigrid is used to solve the global pressure equation, and block ILU is used in the second stage. A sparse black data structure that is compatible with the adaptive implicit method (AIM) is developed and implemented. The preconditioner effectivenss is demontrated using challenging multiphase flow problems with large number of multi-segment wells, for both fully implicit and AIM formulations.

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MS112

Mimetic Discretization Methods on Nonuniform Meshes

We propose a technique for generalizing the Castillo-Grone mimetic schemes on non-uniform meshes based on the application of local transformations and the use of a reference set of cells, RSC. The RSC is not a mesh but a set of two uniform elements that are used while the operators are being built. Contrary to the application of curvilinear coordinates, in our case the differential equation remains the same because we work on the operators instead of transforming the whole equation. We applied this method to construct second and forth order mimetic operators and implemented it to solve boundary-layer like problems. Numerical results show that the implementation of the new operators along with adaptive meshes maintains the same order of accuracy as the Castillo-Grone, uniform operators, while decreasing the convergence-rate constant and maintaining the complexity of the original differential equation.

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MS112

A Fundamental Solution Method For Potencial Flow In Reservoirs With Barriers

An adaptation of the fundamental solution method (MFS) is developed for potential flow in the presence of barriers. Singularities produced by such objects are expressed analytically through the complex variables techniques, and the resultant singular solution is coupled with the MFS. This can be done by the semianalytical nature of the MFS. The numerical results for example problems confirm that the proposed model is an inexpensive, accurate and reliable alternative for computing streamline distributions in two dimensional reservoirs.

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MS112

Modeling of Rupture Propagation Using High Order Mimetic Finite Differences

We present a split node mimetic finite difference method for modeling shear rupture that is consistently fourth-order accurate in its spacial discretization, both in the interior and at the fault. The method called mimetic operator split node (MOSN), uses a staggered grid, and the fault plane is discretized using split nodes for both discontinuous displacements and stress components.

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MS113

Tools for Querying and Comparing Biological Networks

e describe algorithms for two problems related to comparison of biological networks. First, we consider querying problems typified by Given a query pathway Q and a network of interest, does the network contain subnetworks that are similar to Q? The problem is computationally hard, but we significantly extend the class of pathways that can be efficiently queried to the case of trees, and graphs of bounded treewidth. Our algorithm allows the identification of non-exact (homeomorphic) matches, exploiting the color coding technique of Alon et al. The resulting tool, QNet, is used for the first large scale cross-species comparisons of protein complexes. Time permitting, we will also describe a novel framework for the problem of aligning multiple protein networks. At the heart of the framework is a novel representation of multiple networks that is only linear in their size as opposed to current exponential representations. Our alignment algorithm is very efficient, being capable of aligning 10 networks with tens of thousands of proteins each in minutes. (Joint work with Banu Dost, Tomer Shlomi, Nitin Gupta, Eytan Ruppin, Maxim Kalaev, and Roded Sharan)

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MS113

Regulatory Proteins Within a Hierarchical Framework have Distinct Dynamic Properties

Topological properties of social and biological networks have revealed general principles of complex systems. Though recent studies on transcription networks have shown that regulatory proteins could be grouped into layers within a hierarchical framework, the dynamic properties of proteins within and across the layers have not been investigated. Here, we present a novel graph-theoretical algorithm, based on topological sort, to elucidate hierarchical structures in directed networks. We use it to identify three mutually exclusive layers of regulatory proteins - initiators, propagators and effectors - in the yeast transcriptional regulatory program. Overlaying diverse genome-scale datasets on the hierarchical structure reveals the presence of unique dynamic properties characterizing regulatory proteins within each layer. In particular, we show that initiators are present in higher abundance and have a much longer protein half-life but have comparable transcript degradation rates with propagators and effectors. This suggests that post-transcriptional regulation of propagators and effectors is more important than transcriptional regulation. In addition, we find that initiators are significantly noisier than propagators and effectors. This would mean that noisy expression of initiators allows at least few members in a population to readily respond to changes in the environment. At the same time, low noise in effectors and propagators would ensure fidelity in signalling and regulation of relevant target genes. Taken together our findings suggest that regulatory proteins within the hierarchical structure have dynamic properties that are coherent within a layer and distinct across layers, thus making the network more robust and adaptable in a population. Our findings have direct implications in synthetic biology experiments aimed at engineering regulatory networks to control distinct phenotypic outcomes.

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MS113

Examining Biological Networks via Graphlet Degree Signatures

The number of functionally unclassified proteins is large even for simple and well-studied organisms. Methods for determining protein function have shifted their focus from targeting specific proteins based solely on sequence homology to analyses of the entire proteome based on protein-protein interaction (PPI) networks. We design a graph theoretic method demonstrating that in PPI networks, biological function and local network structure are closely related. We apply it to infer biological function of yet unclassified proteins.

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MS113

Host-Pathogen Interactions: Similar Patterns of HIV and P.falciparum

The comparison of interaction networks between the human host, the HIV virus and the malaria parasite P.falciparum shows that both pathogens although distinct in their biology predominantly attack similar targets. In particular, human host proteins are targeted by the pathogens in a non-random and combinatorial manner, allowing them to reach deeply into many functionally diverse protein complexes and functions. Such topological features might represent a general blueprint of host-pathogen systems, allowing a thorough understanding of disease mechanisms.

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MS114

Nonlinear Projective Methods for Solving the Particle Transport Equation

Particle transport problems are difficult to solve, because of their high dimensionality. We will present deterministic methods for solving the multidimensional transport equation on regular and unstructured grids by means of nonlinear projective transport methods. They are based on formulation of special low-order problems coupled with the original high-order transport equation. The structure of low-order equations are particularly attractive for solving multiphysics problems. These methods can be applied for radiative hydrodynamics and nuclear reactor calculations.

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MS114

A Cartesian-grid Based AMR Approach to Simulating Potention Hydrogen Detonations in Reactor Containment Buildings

We present results using a Cartesian grid cut-cell method to simulate potential hydrogen detonations in nuclear reactor containment buildings. Because realistic geometry can be cut directly out of a background Cartesian mesh, cut-cell methods eliminate the need for sophisticated mesh generation tools. However, small computational cells resulting from arbitrary alignment of the geometry with the grid can impose severe stability constraints and compromise accuracy near boundaries. We discuss recent algorithmic advances by Colella, et. al, to address these issues, as well as our experience using EBChombo, an open-source code developed at LBL which implements these recent developments.

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MS114
Computational Foundations for a Fuels Performance Code

The simulation of nuclear reactor fuel performance involves complex thermo-mechanical processes between the fuel pellets, made of fissile material, and the protective cladding barrier that surrounds the pellets. One of the most important design issues for a fuel is to maximize the life of the cladding while maximizing the amount of fissile and waste material consumed within the fuel pellets. In this presentation, we investigate models for the thermo-mechanical response of reactor fuel, which will be used to develop the foundation for a modern fuel performance code.

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MS114
The Need for Predictive Computational Fluid Dynamics in Nuclear Engineering

The impact of computational fluid dynamics (CFD) on nuclear engineering is hindered by our inability to quantify the uncertainty associated with CFD simulations as they are typically performed today. The next generation of CFD must be capable of producing simulations at engineering-required accuracy in a reasonable time and in an automated manner. The purpose of this presentation is to highlight the research topics that are critical to the development of a reliable, timely, and automated CFD capability. In particular, this presentation provides the requirements for verification and validation and uncertainty quantification that will be needed to support a simulation-based design process for nuclear engineering. In addition, the need for and potential impact of solution-based adaptation, high-order discretizations and corresponding solvers and direct integration of CFD with CAD geometry models are discussed.

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MS115
Adaptive Anisotropic Triangulation

We study automatic isotropic adaptive meshes for finite element solution of PDEs. Anisotropic means that the geometric elements need not be shape regular. We show that for problems with discontinuities, anisotropic refinement is more efficient than shape regular refinement. We present an algorithm that achieves an optimal rate of approximation for discontinuous functions in the plane in the L^1 sense. Using N elements, this improves the L^1 error from $O(1/N)$ to $O(1/N^2)$. This is joint work with Juan Carlos Aguillar, Klas Samuelson, and Anders Szepessy.

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MS115
Convergence of Some Adaptive Methods for Nonlinear Geometric PDE

In this lecture, we develop some adaptive numerical methods for a class of nonlinear geometric PDE on 2- and 3-manifolds. Based on some continuous a priori estimates developed in the first part of the talk, we then establish some critical discrete estimates. We then derive a prior and a posteriori error estimates for Galerkin approximations, and describe a class of nonlinear approximation algorithms based on adaptive finite element methods (AFEM). We then establish some new AFEM convergence and optimality results for geometric PDE problems with non-monotone nonlinearities. As an application we consider the constraint equations in the Einstein equations arising in gravitational wave models. We finish by illustrating the algorithms with some examples using the Finite Element ToolKit (FETK).

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MS115
A Posteriori Error Estimators and HP-Adaptivity for Fourth-Order Partial Differential Equations

I will present an extension of a hp-adaptive finite element strategy for second-order reaction-diffusion equations to fourth-order equations using a hierarchical C^1 basis constructed from Hermite-Lobatto polynomials. A priori and a posteriori error estimates will be described, for both the solution at the current order and one order higher. These estimates are used to drive the hp-adaptivity. I will show that the a posteriori error estimates are asymptotically exact on grids of uniform order. Computational results for a linear equation and the Cahn-Hilliard equation will demonstrate estimator accuracy and the reliability of the adaptive strategy

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MS116
Voronoi-Based Binning Techniques: Acceleration

Methods and Applications

In a variety of engineering and physical applications the speed of constructing optimal quantization given the initial set of generators is essential. We present multidimensional generalizations of recently introduced quasi-Newton and multilevel algorithms for the numerical computation of the centroidal Voronoi tessellations. Both algorithms are applied in the context of accelerating binning strategies and compared against most commonly used approaches. Their effectiveness in reducing time and complexity for large-scale image analysis applications is discussed.

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MS116
Computations of Optimal Control Problems for Partial Differential Equations using CVT and POD-based Reduced-Order Modeling

Computing approximations of solutions of nonlinear partial differential equations (PDEs) is a computationally intensive task. For realistic simulations, many thousands or even millions of degrees of freedom are often required to obtain useful approximations. Thus, if one needs to do multiple simulations or to do a simulation in real time, the use of reduced-order modeling (ROM) should be considered. In optimal control or optimization settings, one is faced with the need to do multiple state solves during an iterative process that determines the optimal state and controls. If one approximates the state in the reduced, $d-$dimensional space and if d is small, the the cost of each iteration of optimizer would be very small relative to that using full, high fidelity finite element approximation. We introduce the CVT and POD based reduced order modeling. We focus on how to determine CVT and POD ROM basis using snapshots which one again hopes, can accurately capture the information contained in the snapshot set. Then, we investigate optimal control problems for Navier-Stokes flows.

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MS116
Deployment Algorithms for Multi-Robot Systems Using Voronoi Tessellations

Cooperative robotic networks present new challenges that lie at the confluence of communication, computing, sensing, and control. A lot is known about the individual components of these networked systems, and yet novel theoretical developments are needed to integrate these components into autonomous networks with predictable behavior. The objective of this talk is to present recently developed algorithms for motion coordination of cooperative networks. In our exposition, we pay special attention to the characterization of the correctness, performance, and cost of coordination algorithms. We illustrate our technical approach in algorithms for coverage tasks that make use Voronoi tessellations and Lloyd-type local rules for each agent.

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MS116
Applications of Centroidal Voronoi Tessellation to Logistics System Design

This talk discusses recent applications of centroidal Voronoi tessellation to a couple of logistics system design problems. We proposes computer algorithms to first solve a family of optimal location-allocation problem, and then automatically design discrete vehicle routing zones (VRZ). These logistics problems have significant practical importance, and we utilize a combination of spatial partitioning techniques (e.g., weighted centroidal Voronoi tessellation and disk model).

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MS117
Tensor Decompositions for Text Analysis

This talk presents novel approaches for analyzing text using tensor decompositions. Traditional approaches in text analysis use matrix decompositions, such as the singular value decomposition (SVD). Tensor decompositions consider higher orders than matrices and, thus, allow the analysis to go beyond just terms and documents and enrich the model with additional data types, such as time or language. Illustrative examples will show that this extra information lends itself to a richer interpretation of the data.

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MS117
Fast Newton-Type Methods for Non-Negative Tensor Approximation

Nonnegative Tensor Approximation is an effective decomposition technique that is useful in a wide variety of applications ranging from document analysis and image processing to bioinformatics. There are existing algorithms for nonnegative tensor approximation (NNTA), for example, Lee & Seung's multiplicative updates, alternating least squares, and certain gradient-descent based procedures. However, all these procedures suffer from slow convergence or numerical instabilities. In this talk, I will present improved algorithms for the NNTA problem, which overcome many computational deficiencies of existing methods. In particular, our methods use non-diagonal gradient scaling for faster convergence. These methods provide numerical results that are superior to both Lee & Seung's method as well to the alternating least squares (ALS) heuristic, which is known to work well in some situations but has no theoretical guarantees. I will present experimental results on both synthetic and real-world datasets to demonstrate the effectiveness of the new methods, in terms of better approximations as well as computational efficiency.

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MS117

Spectrum and Pseudospectrum of a Tensor

What is nonlinear spectral theory? A moment's thought indicates that this is just the theory of Lagrange multipliers, which may be viewed as a vast generalization of eigenvalues. However, they are also too general to be as interesting as eigenvalues. We shall examine a special case, multilinear spectral theory, where eigenvalues for tensors can be almost as interesting as matrix eigenvalues, with parallels in multilinear inner-products, tensor norms, hyperdeterminants, Perron-Frobenius theory, pseudospectra, and spectral hypergraphs.

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MS117

Multilinear Projection for Recognition in a Tensor Framework

Multilinear algebra is a principled approach to disentangling and explicitly representing the essential factors (modes) of image formation, among them illumination, scene geometry, and imaging. We develop a multilinear projection algorithm, which is natural for performing recognition in the tensor algebraic framework. Multilinear projection is applied to unconstrained facial image recognition which simultaneously projects an unlabeled face image into multiple constituent mode spaces, where the mode labels are person identity, viewpoint, illumination, etc.

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MS118

Molecular Electron Microscopy to Bio-Physical Modeling and Analysis for Drug Discovery

Human functional processes are mediated through complicated biochemical and biophysical interactions amongst proteins and other biomolecules. A computational understanding of these interactions, as comprehensive as possible, provides important clues for developing therapeutic interventions related to diseases such as cancer and metabolic disorders. In this two part talk I shall first describe a combination of image and geometric processing algorithms to construct spatially realistic structural models of proteins from three dimensional molecular electron microscopy. Subsequently, I shall introduce a new class of algebraic surface spline finite elements, and demonstrate their use in very rapid computation of protein solvation energetics and forces, (based on continuum Poisson-Boltzmann Theory and Generalized Born Theory), and essential for the quantitative analysis of molecular interactions for drug screening and discovery.

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MS118

Accelerating Visual Knowledge Discovery with Query-Driven Visualization

Applying traditional visualization processing techniques to datasets of growing size and complexity has the unfortunate side effect of actually lessening the likelihood of knowledge discovery due to placing an increasingly heavy cognitive burden on the scientific user. One promising approach for better impedance-matching high performance computational machinery with human consumers to maximize likelihood of scientific knowledge discovery is a class of techniques we call "Query-Driven Visualization." This talk will give an overview of Query-Driven visualization and present case studies showing how its favorable computational performance characteristics and its use in a knowledge discovery case study.

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MS118

Visualizing Science at the PetaScale

Scientific visualization is a fundamental data analysis technique for simulation-based research. High performance computing (HPC) systems capabilities are racing far ahead of users' abilities to effectively visualize the data they produce. As petaflop systems produce simulation output of unprecedented scale, it is becoming unfeasible to move these data sets over wide area networks to visualization systems. Achieving the scientific impact of these petascale systems requires scalable visualization tools that aggregate the capabilities of many compute nodes, while rendering the data close to the source, eliminating costly network transfers. This requires remote visualization interfaces to these large-scale visualization systems. The development of the Scalable Collaborative and Remote Visualization Software (SCoReViS) is a direct response to the need for next-generation visualization tools for large-scale HPC platforms and dedicated graphics clusters and is the subject of this talk.

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MS118

Multi-Scale Morse Theory for Science Discovery

Developing advanced techniques for understanding large scale scientific data is a difficult task essential for the success of any supercomputing center. It involves a number of major technical challenges in data management, analysis, and visualization to allow extracting features of unprecedented complexity and dealing with data sets of unprecedented size. Addressing these challenges requires a number of interdisciplinary activities and a tight cycle of basic research, software deployment, and collaboration with the users. In this talk I will present a discrete topological framework for the representation and analysis of large scale science applications. Due to the combinatorial nature of this framework, we can implement the core constructs of Morse theory without the approximations and instabilities of classical numerical techniques. Topological cancellations are then used to build multi-scale representations encompassing local and global trends present in each model. The unique robustness of this approach allows addressing the high complexity of the feature extraction problem for high resolution scientific data. I will demonstrate the effectiveness of this system with the first successful quantitative analysis of two massively parallel simulations. The first is the study of the turbulent mixing layer of hydrodynamic instabilities. The second is the study of the structural properties of porous media under stress and failure.

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PP0

Dirichlet-to-Neumann Method for Acoustic Scattering Applied on Elliptic Grids

We numerically solve the acoustic scattering problem from multiple arbitrarily shaped obstacles in unbounded domains. The domains are made finite by surrounding the regions of interest with artificial boundaries. A non-reflecting boundary condition known as Dirichlet-to-Neumann is applied in conjunction with novel boundary conforming elliptic grids. As a consequence, the computational effort is greatly reduced. The technique is illustrated for scattering of planes waves and line sources from obstacles of various shapes. Advisor: Vianey Villamizar

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PP0

Denserks: A Fortran 90 Library for Adjoint Sensitivity Computations

DENSERKS is a Fortran sensitivity equation solver package designed for integrating models whose evolution can be described by ordinary differential equations (ODEs). A salient feature of DENSERKS is its support for both forward and adjoint sensitivity analyses, with built-in integrators for both first and second order continuous adjoint models. The software implements explicit Runge-Kutta methods with adaptive timestepping and high-order dense output schemes for the forward and the tangent linear model trajectory interpolation. Implementations of six Runge-Kutta methods are provided, with orders of accuracy ranging from two to eight. This makes DENSERKS suitable for a wide range of practical applications. The use of dense output, a novel approach in adjoint sensitivity analysis solvers, allows for a high-order cost-effective interpolation. This is a necessary feature when solving adjoints of nonlinear systems using highly accurate Runge-Kutta methods (order five and above). To minimize memory requirements and make long-time adjoint model integrations computationally efficient, DENSERKS implements a two-level checkpointing mechanism. Several numerical examples are given to illustrate the effectiveness of the implementations.

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PP0

A Computational Series Solution for Unsteady Flow of a Viscoelastic Fluid

In the present work, unsteady flow of a viscoelastic fluid is studied using a recently proposed analytical method named Homotopy Analysis Method (HAM). Using boundary layer theory and similarity transformations, the governing equations reduce into a single highly nonlinear PDE. HAM will be used to find an explicit analytical solution valid in the entire temporal and spatial domain. Finally, the effects of elasticity number, and the time elapsed are studied on the flow characteristics. Advisors: Kayvan Sadeghy, Vahid Esfahanian

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PP0

Developing Parallel, Poly-Algorithms for Integrating Differential Equations

This is an ongoing undergraduate research project on solving differential equations rapidly and accurately using parallel computing, structure of the solution (preconditioning), and a mixed symbolic and numerical computation (poly-algorithms). The underlying difficulty is the coordination and integration of the computational components. We report our efforts on optimizing the interaction of parallel computing and the use of poly-algorithms for an initial value problem for a Riccati equation.

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PP0

Cnoidal Solutions of the Korteweg-de Vries Equation are Linearly Stable

Recent years have seen a lot of activity around the stability analysis of stationary periodic solutions of integrable partial differential equations. We propose a new method for analytically determining these stability spectra. This method relies on the squared-eigenfuction connection between the stability spectrum and the Lax pair spectrum, so often used in the soliton case. We present complete determinations of the spectra of stationary periodic solutions of the Korteweg-de Vries equation. Advisor: Bernard Deconinck, University of Washington

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PP0

RBF-Gegenbauer Reconstruction Methods for Discontinuous Solutions to PDEs

High order approximations of PDEs with discontinuous solutions suffer from a form of oscillatory error known as the Gibbs phenomenon. Radial Basis Functions provide a cheap and simple approximation method, but such approximations are not immune to the Gibbs phenomenon. The Gegenbauer polynomial reconstruction method provides an effective way to remove such oscillations. This work ties Radial Basis Functions and the Gegenbauer postprocessing technique together to produce non-oscillatory solutions to discontinuous problems.

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PP0

AWM - Time-delayed Feedback Control and the Stabilization of Periodic Orbits

Subcritical Hopf bifurcation is a generic mechanism for creating unstable periodic orbits in nonlinear dynamical systems. The Pyragas-type of time-delayed feedback control has been shown to stabilize such orbits when added to the subcritical Hopf normal form. We use analytic and numerical methods of bifurcation theory, developed for Hopf bifurcations in delay differential equations, to investigate an optimal choice for the feedback gain parameters. The results are demonstrated using the Lorenz equations as an example.

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PP0

AWM - Semi-implicit Preconditioning Techniques for Krylov Deferred

We improve the efficiency of the Krylov Deferred Correction (KDC) methods by introducing the semi-implicit preconditioning techniques. The stiff component of the ODE/DAE system is solved by implicit schemes and the nonstiff parts by explicit ones in each deferred correction iteration. Compared with the fully implicit KDC techniques, the SI-KDC techniques improve the efficiency for the same accuracy and stability requirements. The analyses are validated by numerical results.

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PP0

AWM - Gaussian Bounds as they Relate to the 3-D Axisymmetric Navier-Stokes Equations

We study the parabolic equation $u_t+b\cdot\nabla u-\Delta u+\frac{2}{r}\frac{\partial u}{\partial r}=0$, where $(x,t)\in\mathbf{R}^3\times(0,\infty)$, with $x=(x_1,x_2,x_3)$, $r=\sqrt{x_1^2+x_2^2}$ represents the distance to the z-axis, and the term $\frac{\partial u}{\partial r}$ is the directional derivative of u in the direction $e_r=(\frac{x_1}{r},\frac{x_2}{r},0)$. Under the conditions on the drift term that div$b=0$ and $|b|\leq\frac{C}{r}$, for a constant $C>0$, which is weaker than the standard assumption that $|b|\leq\frac{C}{|x|}$, we prove a Gaussian upper bound. With a Gaussian lower bound the approach of Nash would prove regularity.

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PP0

Propagating Modes of Nano-Scale Solid-Fuid Composites

The study is aimed to investigate propagating modes of nano-scale periodic layers of solid-fluid composites with or without damping in the fluid phase. Three-scale homogenization analysis is developed to derive the effective group velocities in analytical forms for the shear-vertical (SV) as well as longitudinal-shear horizontal (P-SH) waves. It is found that propagating modes, i.e. modes with real group velocities may be supported if the viscosity of fluid phase is frequency-dependent. A criterion for the propagating modes is established between the composite medium constants as well as the filling ratio of the fluid phase. The critical filling ratios are given for various solid-water systems.

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PP0

Multigrid Accelerated Nonlinear Diffusion

We always need to solve nonlinear diffusion in MagnetoHydroDynamics simulation. Several iterative solvers have been investigated and their convergences are found to be slow. With the application of multigrid, significant speedup has been observed.

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PP0

On a Connection Between Infinite-Dimensional Linear Dynamic Systems and Nonlinear Differential Equations

We demonstrate a surprising proximity between infinite linear systems of differential equations and nonlinear equations. Besides the analytic results, this approach allows us to obtain a new tool for the computational solution of a broad class of nonlinear equations and scalar conservation laws including Hopf, or inviscid Burgers, equation. The work is done with D.Chae.

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PP0

AWM - Multilevel Approach for Signal Restoration Problems with Structured Matrices

We present a multilevel method for ill-posed problems. In this method we use the Haar wavelets as restriction and prolongation operators. The choice of the Haar wavelet operator has the advantage of preserving matrix structure such as Toeplitz or Toeplitz+Hankel, among grids, which can be exploited to obtain faster solvers on each level. Finally, we present results that indicate the promise of this approach on restoration of signals with edges.

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PP0

A Falling Sphere through Stratified Karo

Settling rates of particles through stratified fluids affect many aspects of life, from air quality to distribution of biomass in the upper ocean. We study the behavior of a sphere falling through a two-layer stratification of miscible, viscous fluid. Motivated by the levitation and velocity reversal found in similar saltwater experiments, we have looked at the effect of the density interface, tank walls, and convection on the settling rate of the sphere. Advisors: Dr. Roberto Camassa, Dr. Richard McLaughlin

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PP0

A Bilinear Immersed Finite Volume Element Method For Diffusion Equations With Discontinuous Coefficients

We present a finite volume element method (FVE) based on the bilinear immersed finite element (IFE) for solving diffusion equations with discontinuous coefficients. This method possesses the usual FVE method's local conservation property and can use a structured mesh or even the Cartitian mesh to solve a boundary value problem whose coefficient has discontinuity along piecewise smooth nontrivial curves. Numerical examples are provided to demonstrate features of this method, including the optimal convergence rate.

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PP0

Rayleigh Waves in Viscoelastic Media

In linear elasticity a Rayleigh wave is a mode which is just at the verge of instability. We examine the question of stability of viscoelastic Rayleigh waves and find that they are also stable if the Poisson ratio is independent of frequency. Otherwise, they can become unstable.

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PP0

Flow Transitions in a Differentially Heated Rotating Channel

We study the transition from steady flow to traveling waves in a differentially heated rotating fluid channel. The fluid is modeled using the Navier-Stokes equations and the transition points are found using linear stability analysis. The dynamics of the fluid near the transition are determined using center manifold reduction and normal forms. The results are then compared to observations made from theoretical and experimental studies of a similar annulus experiment. Advisor: Greg Lewis

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PP0

Multiscale Simulation of 2D Fast Reconnection in a Two-Fluid Plasma

Magnetic reconnection is the breaking and topological rearrangement of magnetic field lines in plasma. Resolving this phenomenon requires resolution of fast waves, which in turn requires numerical computation with short time steps. We consider the GEM (Geospace Environment Modeling) reconnection challenge problem, and compare straightforward computations of fast reconnection with computations that use an accelerated multiscale algorithm. Our algorithm resolves fast waves in isolated regions where reconnection is occurring, while taking larger time steps elsewhere.

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PP0

AWM - Measuring Tumor Blood Flow Parameters Using Contrast-Enhanced Dynamic Image Techniques

The goal of this research is to reduce the time it takes to measure the efficacy of cancer treatments that target tumor blood flow, from a timescale of months to a timescale of weeks or even days, through analyzing time-sequenced data from contrast-enhanced medical imaging techniques to measure the blood flow to a tumor, in lieu of static measurement techniques. Results are shown for a model problem based on real patient data.

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PP0

Multiphase Algorithm and Simulation for MHD of Ablated Materials

A numerical algorithm for the simulation of magnetohydrodynamics in conducting liquids and partially ionized gases is presented. For the hydro part, the nonlinear hyperbolic conservation laws with electromagnetic terms are solved using Godunov-type Riemann solvers and techniques developed for free surface flows; for the electromagnetic part, the electrostatic approximation is applied and an elliptic equation for electric potential is solved by embedded boundary method. Atomic processes in the ablated material and the ExB drift motion due to cloud charging have been incorporated in the model. The code has been applied to simulations of the pellet ablation in a magnetically confined plasma, the expansion/distortion of a mercury jet in magnetic fields, and magnetically controlled plasma plume expansion.

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PP0

AWM - A Overset Grid Method for the Study of Human Tear Film

Human tear film is a multilayer structure playing a vital role in the health and function of the eye. Using lubrication theory, we model the evolution of the tear film over a blink cycle. The highly nonlinear governing equation is solved on an overset grid by method of lines coupled with finite differences. Comparisons with in vivo measurements show quantitative and qualitative agreement under partial blink and reflex tearing conditions, respectively.

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PP0

The Search Kinetics of a Target Inside the Cell Nucleus

We obtain new estimates for the mean search time of a transcription factor (TF) or an enzyme to find a target in a cell nucleus. The search switches between one-dimensional motion along the DNA molecule and free Brownian motion in the entire crowded nucleus. We give analytical expressions for the mean time τ_{DNA} the particle stays on the DNA molecule and the mean time τ_{free} it diffuses freely. Contrary to previous results, but in agreement with experimental data, we find a factor $\tau_{DNA} \approx 5\tau_{free}$ for the Lac-I TF. We also show that a higher DNA density leads to a more efficient search process.

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PP0

AWM - Mathematical Modeling of Disease and Competition Dynamics in Metapopulations with Applications to Barley Yellow Dwarf Virus

Non-native grasses have been invading and displacing native perennial grasses in much of the western United States. One possible factor influencing invasion is the barley yellow dwarf virus. We model and analyze the dynamics of multi-host pathogen and vector communities by using coupled systems of ordinary differential equations to understand how the forces of interspecific infection between multiple species infected by a single pathogen combine with metapopulations to allow invasion by exotic species.

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PP0

Parameter Sensitivity Investigation of a Mathematical Model of Glioma Tumorigenesis Mediated by Platelet-Derived Growth Factor

We present a reaction-diffusion model based upon data from experimental rat models of glioma tumorigenesis collected by Professor Peter Canoll. Using a sensitivity analysis technique incorporating latin hypercube sampling (LHS) and partial rank correlation coefficients (PRCC), we show that the two most influential parameters upon the ratio of uninfected progenitor cells to total progenitors comprising the tumor are the proliferation rate of infected progenitors and the rate of consumption of PDGF by uninfected progenitors. Advisers: Kristin R. Swanson, Peter Canoll

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PP0

A Model for Particle Size Segregation in Granular Flow Under Nonuniform Shear

A hyperbolic conservation law in one space variable and time describes particle size segregation in the presence of nonuniform shear. This PDE generalizes the Savage-Lun (1988) and Gray-Thornton (2005) models of segregation in granular avalanches, which assume uniform shear. Size segregation is observed in a Couette cell experiment in which a bidisperse mixture of spherical glass beads is sheared by rotating the bottom boundary. Experimental results are compared to analysis of the PDE model.

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PP0

AWM - Optimal Control Applied to Native-Invasive Population Dynamics

An ODE system modeling interactions between invasive and native species is presented. Disturbance in the system is modeled as a control variable in the growth terms. An objective functional is formulated to maximize the native species while minimizing the cost of implementing the control. A new existence result for an optimal control in the case of quadratic growth functions is given. Numerical results provide suggestions for managing the disturbance regime when invasive species are present.

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PP0

Thin Film Evolution over Thin Porous Layers

We study the simulated models of the aqueous layer on the pre-corneal tear films of a human eye. These models describe the behavior of fluid films with and without the inclusion of the permeable porous medium that models a contact lens. A fluid dynamic model for the thin fluid film over thin porous layers is formulated by using a nonlinear fourth order partial differential equation with four boundary conditions and one initial condition. The evolution equations are solved numerically in Matlab in order to predict the effect of various parameters (at realistic values) on time of the thin films rupture. The results indicate that the presence of thin porous layers is a dominant effect and the different slip conditions at the liquid-lens boundary also have significant impact on thinning the thin aqueous layers. The computed numerical results allow us to predict film break up times for tear films on a contact lens. Advisor: Dr. Daniel M. Anderson

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PP0

Accurate Computations of Accelerator Cavity Frequencies Using VORPAL

Accurate frequency estimation of electromagnetic resonant cavities is crucial to the design of the future generation of particle accelerators. We describe an efficient Finite Difference Time Domain (FDTD) approach for frequency extraction that relies on a small number of simulations and post-processing using the SVD algorithm with Tikhonov regularization. Recent results using the parallel FDTD code, VORPAL, illustrate the ability to produce frequencies that are within 0.0125% of experimental measurements after accounting for manufacturing errors.

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PP0

Phase Separation Dynamics in Multicomponent Alloys

Our topic is mathematical models describing pattern formation and phase separation/transition within multicomponent metal alloys – specifically, we are studying the Cahn-Morral system of partial differential equations, a phenomenological model for these phenomena. We use numerical bifurcation and continuation to study equilibria for the system in one and two dimensions. This allows us to understand the behavior seen in simulations. We also describe our numerical method.

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PP0
AWM - Optimal Movement in the Prey Capture Behavior of Weakly Electric Fish

The black ghost knifefish is modeled as a solid rigid ellipsoid in an ideal fluid. Prey capture is treated mathematically as a constrained optimization problem: minimize the cost function (which is a function of the applied forces and torques) subject to a set of constraints that includes Kirchhoff's equations of motion and initial and final conditions matched to videotaped trajectories of the fish. Results show that actual fish trajectories are very similar to optimal trajectories.

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PP0
Mathematical Modeling of Wall Street Randomness and Measure

Often stochastic differential equations (SDEs) are used to model Wall Street randomness in relation to moving average share prices, price earnings and book values. A form of stochastic differential equations (SDEs) is being proposed here to study governing quantities such as M and S which is the ratio of an exponentially weighted moving average of a share price to the share price itself and price earnings ratio with book values respectively. The SDEs for other path-dependent random variables will also be derived if appropriate quantities can be correlated with the moving averages. We will present the mathematical modeling methodology for the expected exit and entrance time and the cumulative distribution function for the first exit time with respect to certain class of funds and type of industry in the stock market analysis. The boundary conditions for these equations will be discussed in some depth. Some numerical solutions of the SDEs will also be presented. We will consider the crossing of two moving averages price earnings ratio with the book value for different weights. The application to the pricing of path dependent options will also explored.

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PP0
Postprocessing Global High Order Approximation Methods

Global High Order (Pseudospectral and Radial Basis Function) Approximation Methods applied to piecewise continuous functions exhibit the well-known Gibbs phenomenon. We examine and compare known methods to remove the Gibbs oscillations and present a collection of Matlab programs that implement the methods. The software features a Graphical User Interface that allows easy access to the postprocessing algorithms for benchmarking and educational purposes. Some results on benchmark problems are examined.

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PP0
AWM - Using IMSCAND to Extract Clusters from Data with Multiple Similarity Measures

We are considering a higher-order analogue of the matrix singular value decomposition (SVD), called CANDECOMP/PARAFAC (CP). Our approach exploits the structure of the two-dimensional slices, which are formed from the product of a sparse matrix and its transpose. Though the full slices are dense, we only form them implicitly, storing only the sparse matrix factors. Based on this tensor representation, we present a new tensor decomposition called Implicit Slice Canonical Decomposition (IMSCAND), which is equivalent to the CP.

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PP0
Minimizing the Kohn-Sham Equation: Adaptive Parmater Selection

The electronic ground state of a system can be computed by minimizing the Kohn-Sham total energy functional and solving for the wavefunctions, which allow for the determination of electronic properties of materials. We analyze and compare the Self-Consistent Field (SCF) iteration, the direct constrained minimization (DCM) algorithm, and the trust region DCM, algorithms designed to minimize this function. We develop and test rules for adaptively selecting parameter values in each algorithm to improve convergence rates.

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PP0

AWM - Characterizing the Cortical Folding Pattern Across Species Using Prolate Spheroidal Harmonics

The human cerebral cortex is a highly folded surface. How these folds occur, and their significance, has fascinated scientists across a variety of disciplines. My research aims to answer some of these questions by using a Turing reaction-diffusion system on a prolate spheroidal domain and seeing how domain size and shape play a key role in cortical patterning across different mammalian species.

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PP0

Elastic Scattering From Viscous Incompressible Fluid Objects at High Reynolds Number

We use singular perturbation techniques to compute the scattering cross-section for an incident plane compressional wave propagating in an elastic medium scattered by spherical and cylindrical inclusions filled with fluids at high Reynolds number, where the spherical and cylindrical inclusions are assumed to have radii much less than the wavelength of the incoming wave. Advisor: Vianey Villamizar

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PP0

Identifying Sociological Trends in Facebook Networks

With real-world social connections spilling over into the digital domain, online social networks provide information about underlying real world ties. Using variants of eigenvector-based methods for community detection [M. Newman, Phys. Rev. E 74, 036104 (2006)], we identify communities of pages/individuals in Facebook networks restricted to individual schools and compare against a collection of characteristics provided by each individual. We additionally identify communities in corresponding gender-restricted networks, comparing with the overall networks and characteristics. Advisors: Dr. Peter J. Mucha, Dr. Mason A. Porter

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PP0

Ellis Model of Thin Film Flow: Dynamics and Stability

Shear-dependent rheology's influence on the temporal stability of an Ellis fluid flowing down an inclined plane is examined using a numerical approach based on a generalized Orr-Sommerfeld eigenvalue problem. Further, a non-linear evolution equation for the film thickness is found from long-wave theory. Existence of permanent waves and periodic numerical solutions are explored. The shape and amplitude of long-time waveforms are influenced by non-Newtonian rheology.

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PP0

Acceleration of Time Integration: Experiments with One-Dimensional Advection

We investigate one-dimensional pure advection to test methods of maintaining fast time integration with increasing spatial resolution. We demonstrate three complementary techniques for accelerating time integration: 1) high-order single-step time integration, both explicit and implicit; 2) compact implicit time integration with unconditional stability in Courant number; and 3) single-cycle multi-grid linear solvers. We present performance and accuracy results for various combinations of these techniques over a wide range of Courant numbers.

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PP0

Exploring Non-Linear Dynamical Systems by Markov Chain Monte Carlo

Monte Carlo methods are very important in computational physics, physical chemistry, and related applied fields, and have diverse application. We will introduce Markov chain Monte Carlo (MCMC) as an anatomical tool for nonlinear dynamical systems. Sampling over initial conditions, we can find "special solutions" which satisfy a given condition. We investigate invariant sets, periodic orbits and bifurcation structures in chaotic dynamical systems.

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PP0

Fourier analysis of multigrid methods on hexagonal

grids

This paper applies local Fourier analysis to multigrid methods on hexagonal grids. Using oblique coordinates to express the grids and a dual basis for the Fourier modes, the analysis proceeds essentially the same as for rectangular grids. The framework for one- and two-grid analysis is given, and then applied to analyze the performance of multigrid methods for the Poisson problem on a hexagonal grid. Numerical results confirm the analysis.

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PP0

AWM - Compact Conservative Jacobians on Rectangular and Hexagonal Grid

In this talk, we will prove that there is no conservative compact symmetric approximation of order greater than two for the two-dimensional non-divergent incompressible barotropic equation on a uniform rectangular grid or hexagonal grid. However, we will give noncompact conservative fourth-order discretizations on both grids and corresponding compact conservative discretizations for the boundary points.

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