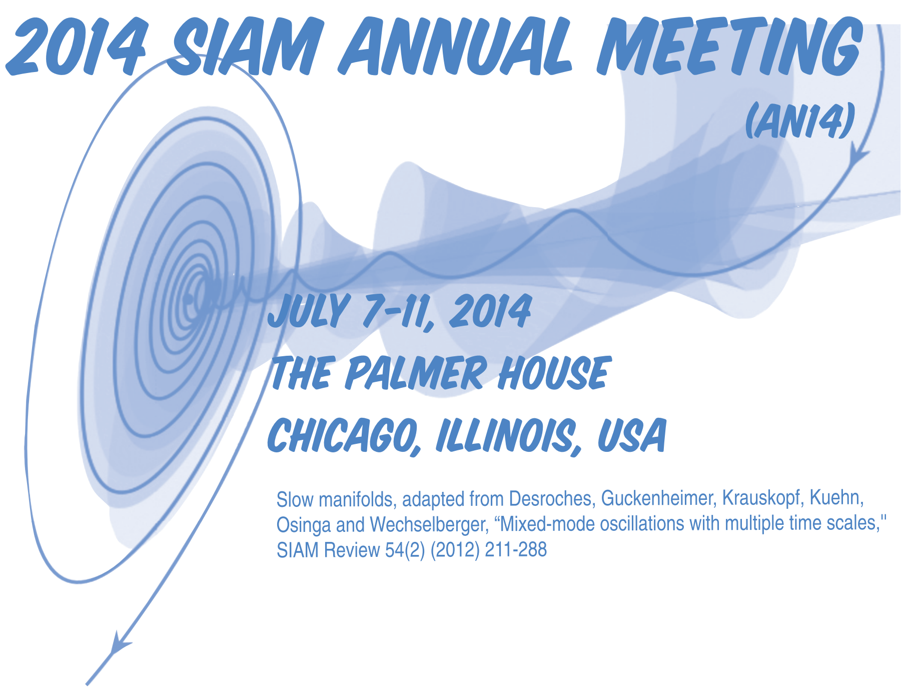
AN4 Abstracts



Slow manifolds, adapted from Desroches, Guckenheimer, Krauskopf, Kuehn, Osinga and Wechselberger, "Mixed-mode oscillations with multiple time scales," SIAM Review 54(2) (2012) 211-288

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IC1

Equilibrium Analysis of Large Populations Dynamics

The first part of the talk will review several applications, including bird flocking, information percolation in social networks, valuation of exhaustible resources, high frequency market making, emissions regulation, , for which models of large populations dynamics can be brought to bear. These models will be framed in the context of the theory of mean field games. The second part of the talk will present recent equilibrium existence results, and discuss some of the nagging computational challenges raised by the need for reasonable numerical approximations to these equilibria.

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IC2

Solving Stochastic Inverse Problems Using Sigma-Algebras on Contour Maps

We describe recent work on the formulation and numerical solution of stochastic inverse problems for determining parameters in differential equations with stochastic data on output quantities. The new approach involves approximating the generalized contour maps representing set-valued inverse solutions, using the approximate contour maps to define a geometric structure on events in the sigma-algebra for the probability space on the parameter domain, and exploiting the structure to define and approximate probability distributions in the space. We will present various examples, including high-dimensional problems involving spatially varying parameter fields in storm surge models.

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IC3

Computational Biology in the 21st Century: Making Sense out of Massive Data

The last two decades have seen an exponential increase in genomic and biomedical data, which will soon outstrip advances in computing power to perform current methods of analysis. Extracting new science from these massive datasets will require not only faster computers; it will require smarter algorithms. We show how ideas from cutting-edge algorithms, including spectral graph theory and modern data structures, can be used to attack challenges in sequencing, medical genomics and biological networks.

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IC4

The Evolution of Combinatorial Solvers for Laplacian Linear Systems

Fast solvers that are based on combinatorial techniques have been investigated for more than two decades now. The most successful of these (at least theoretically) solve symmetric diagonally linear systems, a class that includes Laplacians of graphs. The talk will describe these techniques, starting with Vaidya's 1991 solver and ending with very recent algorithms by Kelner and others. The talk will focus on how the graph-matrix isomorphism is used in these solvers, on the class of matrices that they can be applied to, and on the gap between theory and practice in this area.

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IC5

Optimization Algorithms for Machine Learning

The extraordinary success of search engines, recommendation systems, and speech and image recognition software suggests that future advances in these technologies could have a major impact in our lives. In this talk, we discuss modern intelligent-algorithmic systems based on sophisticated statistical learning models and powerful optimization techniques. One can envision new algorithms that operate in the stochastic or batch settings, and that take full advantage of parallelism. We review our remarkable understanding of classical stochastic approximation techniques, and pose some open questions. The lecture concludes with a discussion of modern neural nets and the demands they impose on optimization methods.

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IC6

The Mathematical Problems of Isotropic-Nematic Interface

Liquid crystals represent a vast and diverse class of anisotropic soft matter materials which are intermediate between isotropic liquids and crystalline solids. The various liquid crystal phases can be characterized by the type of ordering,one of the most common liquid crystal phases is the isotropic phase, another is the nematic phase. In this talk, a wide spectrum of mathematical problems of isotropic-nematic interface will be considered. One set of problems to be considered is the relationship between these different levels of modeling, for example how one can make a rigorous passage from molecular/statistical descriptions to continuum theories. Special consideration will be given to the existence, uniqueness and regularity of the solutions of the Landau-de Gennes theory.

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IC7

The Statistics Behind the Discovery of the Higgs Boson

The standard model of particle physics is a wildly successful theory of fundamental particles and their interactions. The Higgs boson is a particle that was predicted nearly 50 years ago to address a serious theoretical consistency issue in the Standard Model of particle physics, but it has never been observed. The Large Hadron Collider is a multi-national, multi-billion dollar experiment to search for the Higgs boson and other new phenomena. I will discuss the statistical aspects of the recent discovery of the Higgs boson, including the collaborative statistical modeling of the data and the statistical procedures we employ. With multi-petabyte datasets and complex statistical models, we are arguably pushing a frontier of statistical analysis and quickly outstripping our most advanced tools.

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IC8

Random Braids

Braids are mathematical objects closely related to knots. They consist of a set of strings embedded in three dimensions, anchored at both ends. Plotted in a spacetime diagram, trajectories of two-dimensional systems naturally form braids. When the trajectories correspond to periodic orbits they form closed braids, and there are powerful mathematical techniques available to analyze the dynamics. If the trajectories are chaotic, then the analysis is not so simple. I will describe the types of braids that arise when dealing with chaotic orbits, and discuss their connection to surface dynamics. I will also discuss applications to sparse trajectory datasets.

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IP1

Age of Networks

Networks are becoming increasingly relevant in a host of domains. In the tech industry, we see the Internet, the WWW, and many online social networks. In economics, we are experiencing both the positive and negative effects of a global networked economy. In biomedical applications, the structure of gene regulatory networks is relevant for the treatment of many human diseases. In this talk, I describe quite generally models we are using to describe these networks, processes we are studying on the networks, algorithms we have devised for the networks, and finally, methods we are developing to indirectly infer network structure from measured data. I then focus on a couple of specific applications, including one to cancer genomics.

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IP2

Big Data, Sparse Information: Bayesian Inference for Large-scale Models, with Application to Inverse Modeling of Antarctic Ice Sheet Dynamics

Predictive models of complex geosystems often contain numerous uncertain parameters. Rapidly expanding volumes of observational data present opportunities to reduce these uncertainties via solution of inverse problems. Bayesian inference provides a systematic framework for inferring model parameters with associated uncertainties from (possibly noisy) data and prior information. However, solution of Bayesian inverse problems via conventional MCMC methods remains prohibitive for expensive models and high-dimensional parameters. Observational data, while large-scale, typically can provide only sparse information on model parameters. Based on this property we design MCMC methods that adapt to the structure of the posterior probability and exploit an effectively-reduced parameter dimension, thereby rendering Bayesian inference tractable for high-dimensional Antarctic ice sheet flow inverse problems.

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IP3

Pattern Recognition with Weakly Coupled Oscillatory Networks

One outstanding property of biological neural networks is the ability to perform pattern recognition tasks. To mimic this property with a man-made device that processes information in parallel has been a great challenge. Traditional approaches employ many interconnected units and are inherently difficult to construct. In the lecture, we will focus on neural network models of weakly coupled oscillators with time-dependent coupling. In these models, each oscillator has only one or a few connections to a common support, which makes them predestinated for hardware implementation. We will discuss the dynamics of different network architectures, compare their scalability, present experimental realizations of the networks and point out open challenging mathematically problems.

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IP4

Scientific Computing in Movies and Virtual Surgery

New applications of scientific computing for solid and fluid mechanics problems include simulation of virtual materials for movie special effects and virtual surgery. Both disciplines demand physically realistic dynamics for such materials as water, smoke, fire, and brittle and elastic objects. These demands are different than those traditionally encountered and new algorithms are required. This talk will address the simulation techniques needed in these fields and some recent results including: simulated surgical repair of biomechanical soft tissues, extreme deformation of elastic objects with contact, high resolution incompressible flow, clothing and hair dynamics. Also included is discussion of a new algorithm used for simulating the dynamics of snow in Disneys animated feature film, "Frozen".

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IP5

Big Data Visual Analysis

We live in an era in which the creation of new data is growing exponentially such that every two days we create as much new data as we did from the beginning of mankind until the year 2003. One of the greatest scientific challenges of the 21st century is to effectively understand and make use of the vast amount of information being produced. Visual data analysis will be among our most important tools to understand such large and often complex data. In this talk, I will present state-of-the-art visualization techniques, including ways to visually characterize associated error and uncertainty, applied to Big Data problems in science, engineering, and medicine.

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IP6

Virtual Electrophysiology Laboratory

We present the development of a highly innovative patient-specific MRI-based heart modeling environment that represents cardiac functions from molecular processes to electrophysiological and electromechanical interactions at the organ level. This environment is termed "virtual electrophysiology lab". We present our attempts to translate this environment into the clinic and apply it to the non-invasive diagnosis and treatment of heart rhythm and contractile disorders in patients with structural heart disease. This pioneering effort offers to integrate, for the first time, computational modeling of the heart, traditionally a basic-science discipline, within the milieu of contemporary patient care. The robust and inexpensive non-invasive approaches for individualized arrhythmia risk stratification and guidance of electrophysiological therapies presented here are expected to lead to optimized therapy delivery and reduction in health care costs.

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IP7

Unilever, Science and eScience: The Challenges Ahead

Unilever is a large multinational and a market leader in the fast moving consumer goods business, with well known products in the sectors of home care, personal care, refreshments and foods. We are embracing new ways of doing R&D to deliver bigger, better, faster innovations to market. The digital revolution, eScience, is already permeating everything we do at home: how could we pay our bills without eBanking, connect with our friends without Facebook, or find our way around without SatNav? The same revolution is helping us move faster at work. But how can we make this digital eScience revolution work for us?

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IP8

Evolutionary or Revolutionary? Applied Mathematics for Exascale Computing

The move to exascale computing is expected to be disruptive due to significant changes in computer architectures. Advances in applied mathematics will be necessary to realize the full potential of these supercomputers, but will these advances be incremental changes to existing methods or will exascale computing require a substantial rethinking of how we compute? To answer this question, the DOE Advanced Scientific Computing Research Program chartered a working group, which Dr. Hittinger co-chaired. In this talk, he will discuss the findings of the working group: the opportunities for new applied mathematics research that will enable exascale computing. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-645318.

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IP9

Physics-based Animation Sound: Progress and Challenges

Decades of advances in computer graphics have made it possible to convincingly animate a wide range of physical phenomena, such as fracturing solids and splashing water. Unfortunately, our visual simulations are essentially "silent movies" with sound added as an afterthought. In this talk, I will describe recent progress on physics-based sound synthesis algorithms that can help simulate rich multi-sensory experiences where graphics, motion, and sound are synchronized and highly engaging. I will describe work on specific sound phenomena, and highlight the important roles played by precomputation techniques, and reduced-order models for vibration, radiation, and collision processing.

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SP1

AWM-SIAM Sonia Kovalevsky Lecture: The Evolution of Complex Interactions in Non-Linear Kinetic Systems

Recent developments in statistical transport modeling, ranging from rarefied gas dynamics, collisional plasmas and electron transport in nanostructures, to self-organized or social interacting dynamics, share a common description based in a Markovian framework of birth and death processes. Under the regime of molecular chaos propagation, their evolution is given by kinetic equations of non-linear collisional (integral) Boltzmann type. We will present an overview of analytical issues and novel numerical methods for these equations that preserve the expected conserved properties of the described phenomena, while enabling rigorous stability, convergence and error analysis.

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SP2

Fast, Accurate Tools for Physical Modeling in Complex Geometry

During the last two decades, fast algorithms have brought a variety of large-scale physical and biophysical modeling tasks within practical reach. This is particularly true of integral equation approaches to electromagnetics, acoustics, gravitation, elasticity, and fluid dynamics. The practical application of these methods, however, requires analytic representations that lead to well-conditioned linear systems, quadrature methods that permit the accurate evaluation of boundary integrals with singular kernels, and techniques for a posteriori error estimation that permit robust mesh refinement. I will give an overview of recent progress in these areas with a particular emphasis on wave scattering problems in complex geometry.

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SP3

W. T. and Idalia Reid Prize in Mathematics Lecture: On the Master Equation in Mean Field Theory

One of the major founders of Mean Field Games, P.L. LIONS has introduced in his lectures at College de France the concept of Master Equation. It is obtained through a formal analogy with the set of partial differential equations derived for the Nash equilibrium of a differential game with a large number of players. The objective of this lecture is to explain its derivation, not by analogy, but through its interpretation. We do that for both Mean Field Type Control and Mean Field Games. We obtain complete solutions in the linear quadratic case. We analyze the connection with Nash equilibrium.

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SP4

I. E. Block Community Lecture: Search and Discovery in Human Networks

In the past few years, we have seen a tremendous growth in public human communication and self-expression, through blogs, microblogs, and social networks. In addition, we are beginning to see the emergence of a social technology stack on the web, where profile and relationship information gathered by some applications can be used by other applications. This technology shift, and the cultural shift that has accompanied it, offers a great opportunity for computer scientists, artists, and sociologists to study (and organize) people at scale. In this talk I will discuss how the changing web suggests new paradigms for search and discovery. I will discuss some recent projects that use web search to study human nature, and use human nature to improve web search. I will describe the underlying principles behind these projects and suggest how they might inform future work in search, data mining, and social computing.

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SP5

Julian Cole Lecture: Growth, Patterning, and Control in Nonequilibrium Systems

Dense-branching morphologies are among the most common forms of microstructural patterning in systems driven out of equilibrium. Prediction and control of the emergent patterns are difficult due to nonlocality, nonlinearity and spatial heterogeneity. Focusing on viscous fingering in a circular Hele-Shaw cell as a paradigm for such phenomena, we use theory and numerics to demonstrate that by controlling the injection rate of the less viscous fluid, we can precisely suppress the evolving interfacial instabilities and control the shape of growing bubbles. Experiments confirm the feasibility of the control strategy. Extensions to other pattern-forming systems will be discussed.

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SP6

Theodore Von Karman Prize Lecture: Materials from Mathematics

We present examples of new materials whose synthesis was guided by some essentially mathematical ideas from pde and the calculus of variations. These materials undergo phase transformations from one crystal structure to another, without diffusion. The underlying mathematical theory was designed to identify alloys that show exceptional reversibility of the transformation. The new alloys do show unprecedented reversibility, but raise fundamental new questions for theory. Some of these alloys convert heat to electricity (without a separate electrical generator), and provide an interesting possible route to recover the vast amounts of energy stored on earth at small temperature difference. The lecture will be mathematically/experimentally nontechnical and suitable for a broad audience. (http://www.aem.umn.edu/ james/research/)

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CP1

Filtering Algorithm For Pod-Based Reduced Order Modeling Techniques

Principal component analysis (PCA) is a technique that can be used to determine the most important components on a set of varying data. PCA algorithms produces statically independent score variables that determines the importance of each component. In this manuscript, we introduce a new filtering algorithm that can be used to down-select a smaller number of directions from the POD-determined basis in order to render a more effective reduction of dimensionality. The error resulting from this filtering can be upper bounded using a randomized range finding algorithm (RFA), employed in some of our previous developments. A neutron transport model is used to demonstrate the proof of principle and exemplify the implementation and mechanics of the proposed algorithm. The proposed algorithm can be classified as a PCA algorithm, yet, it uses the error metric associated with the RFA to generate a set of principal components with a certain probability.

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CP1

An Efficient Output Error Bound for Reduced Basis Methods Applied to Parametrized Evolution

Equations

We present an efficient a posteriori output error bound for the reduced basis method applied to nonlinear parameterized evolution equations. With the help of a dual system and a simple representation of the residual in the primal system, the output error can be estimated sharply. Such an error bound is successfully applied to reduced order modeling of nonlinear chromatography, and the underlying optimization can be solved efficiently using the reduced model.

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CP1

Employing Non-Converged Iterates for Reduced Order Modeling

Recently, reduced order modeling (ROM) is being used in various engineering fields. Model-specific basis can be constructed utilizing a randomized range finding algorithm (RFA) where snapshots of the models response are used to construct the basis. However, this process might be computationally taxing. This work proposes an algorithm that utilizes the non-converged iterates of the model of interest to construct the basis. A mathematical proof showed that the resulting subspace in equivalent to that constructed using the converged snapshots. The two subspaces were compared numerically in terms of the dominant angle and an error metric that has been developed in a previous work. Results indicate that the proposed algorithm produces a subspace that is representative and inclusive of the subspace obtained by the converged snapshots.In addition to that, a numerical test is implemented to illustrate the application of the proposed algorithm in nuclear engineering design calculations.

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CP1

Using Snapshots of the Derivatives in Proper Orthogonal Decomposition (POD)-Based Reduced Order Methods (ROM) for Dynamical Systems

POD-based ROM methods use solution snapshots (SS) or snapshot difference quotients. We explore a POD ROM method that, apart from SS, also uses time derivative snapshots (TDS), calculated from the right-hand side of the dynamical system. In general, TDS do not belong to the span of the SS. We develop error estimates, supported by numerical tests, suggesting that a ROM utilizing both TDS and SS approximates the solution better than one based only on SS.

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CP1

Adaptive Proper Orthogonal Decomposition Reduced Order Models Via Incremental SVD

Meeting approximation error tolerances may require global reduced order models (ROMs) with unacceptably large numbers of ROM basis vectors. To overcome this problem, adaptive sampling and incremental singular value decomposition are used to construct smaller, locally accurate proper orthogonal decomposition (POD) ROMs. Replacing a global POD ROM with a collection of local POD ROMs generally reduces approximation error for a fixed number of ROM basis vectors.

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CP1

Robust Reduced-Order Models Via Fast, Low-Rank Basis Updates

The large computational cost associated with high-fidelity physics-based simulations has limited their use in practical situations. Model Order Reduction (MOR) is an attempt to reduce the computational cost of such simulations by approximating the solution in well-chosen, low-dimensional affine subspaces. Recent developments in nonlinear MOR theory that achieves increased parametric robustness and additional speedup using fast, online reduced-basis updates will be presented. These new techniques will be demonstrated on parametric, large-scale, 3D fluid mechanical problems.

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CP2

Two-Point Riemann Problem for Inhomogeneous Conservation Laws: Geometric Construction of Solutions

We consider the following conservation law: $\partial_t u(x,t) + \partial_x f(u(x,t)) = g(u)$ The following boundary conditions are specified: $u(0-0,t) = u_{0-}$ and $u(X+0,t) = u_{X+}$. In addition, we specify the initial condition $u(x,0) = u_{x0}$ for $x \in (0,X)$. Method of characteristics is used to show the evolution of the initial profile and the discontinuities at the boundaries as well as appearance and in some cases disappearance of internal discontinuities. For illustration purposes the function $f(u)$ will be assumed to have 3 critical points.

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CP2

On Eigenfunction Expansion Solutions for the Start-Up of Fluid Flow

Textbooks describe the process of "subtracting off' the steady state of a linear parabolic PDE as means for obtaining a homogeneous BVP to solve by eigenfunction expansions. While this works for the start-up problem for a Newtonian fluid between parallel plates, it leads to erroneous solutions to the corresponding problem for a class of non-Newtonian fluids. We show this is due to non-rigorous enforcement of the start-up condition, violating the principle of causality.

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CP2

Transport in Confined Structures As a Multiscale Problem and Numerical Results for Nanopores

Charge transport through confined structures such as nanopores differs from transport in bulk. Confined structures give rise to multiscale problems; more precisely, transport and scattering occur in the longitudinal direction, while the particles are confined in the two transversal directions. We have derived a conservation law of the form $\partial_t \rho(x,\eta,t) + \partial_x F^x(x,\eta,t) + \partial_\eta F^\eta(x,\eta,t) = 0$ from the Boltzmann equation, where ρ is the concentration, η is energy, and F^x and F^η are fluxes given explicitly by the harmonic confinement potential. We also present several recent numerical results for artificial nanopores and for ion channels such as certain antibiotics.

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CP2

A Free Boundary Approach for Solving a Two-Dimensional Riemann Problem for the Isentropic Gas Dynamics Equations

We consider a two-dimensional Riemann problem for the isentropic gas dynamics equations modeling strong (or transonic) regular reflection. We write the problem in self-similar coordinates and obtain a free mixed boundary problem for the reflected shock and the subsonic state behind the shock. Using the theory of 2nd order elliptic equations with mixed boundary conditions as well as various fixed point arguments, we prove existence of a solution to the above Riemann problem in a neighborhood of the reflection point.

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CP2

Singular Behavior of the Navier Stokes Flow Through a Non-Convex Polyhedral Cylinder

This result is a mathematical background to solve the compressible flow near the sharp edge. We consider the compressible viscous Navier-Stokes equations in a non-convex polyhedral cylinder. We split the edge singularity occurring at the non-convex edge from the velocity vector and show the high regularity for the velocity remainder. The local sound wave is propagated into the region along the streamline emanated from the non-convex edge and its derivatives blow up across the streamline.

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CP2

Higher Order Analyses of Laminated Composite Shells and Plates

The free Vibration analyses of laminated cylindrical shells by using higher order shear deformation theories. Equilibrium equations are formulated using the equations of stress resultants to attain a system of differential equations and are solved for free vibrations. Boundary conditions considered are simply supported and lamination is cross ply. The third orders shear deformation theory of that considers transverse normal stress, shear deformation and rotary inertia has been developed and used. An exact analytical solutions and boundary condition of shell has been obtained. The (first five) natural frequency parameters are reported and compared with previously published research using a first order approximation. Results are also compared with an accurate 3D finite element analyses.

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CP3

Pushing and Showing in Hallways and Doorways

We investigate the location of macroscopic equilibrium states, both stable and unstable, in systems of interacting particles, modelling the evolution of flocks, swarms and pedestrian crowds constrained by walls and obstacles. Unstable equilibrium states provide valuable information about qualitative system behaviour, boundaries between stability regions, and transitions between modes of flow. Equation-free methods connecting macroscopic and microscopic descriptions are employed to perform analysis and parameter continuation of equilibria and bifurcation points.

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CP3

Spatial Localization in Heterogeneous Systems

We study spatial localization in the generalized Swift-Hohenberg equation

$$u_t = r(x)u - (1 + \partial_{xx})^2 u + N(u)$$

with either quadratic-cubic or cubic-quintic nonlinearity $N(u)$ subject to spatially heterogeneous forcing through the spatially varying parameter $r(x)$. Different types of forcing with different spatial scales are considered and the corresponding localized structures are computed. The results indicate that spatial heterogeneity exerts a significant influence on the location of spatially localized structures in both parameter space and physical space, and on their stability properties. The results are expected to assist in the interpretation of experiments where departures from spatial homogeneity are unavoidable.

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CP3

Billiard Dynamics of Bouncing Dumbbell

A system of two masses connected with a weightless rod(called dumbbell) interacting with a flat boundary is considered. The sharp bound on the number of collisions with the boundary is found using billiard techniques. In case the ratio is large and the dumbbell rotates fast, an adiabatic invariant is obtained.

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CP3

Solitary Waves and the N-particle Algorithm for a Class of Euler-Poincaré Equations

Nonlinearity arises generically in mathematical models of physical phenomena, and the interplay between nonlinearity and dispersion is thought to be responsible for many of these phenomena, such as the existence of traveling waves. We explore the relation between nonlinearity and dispersion by studying the N-particle system of the Euler-Poincaré differential equations, or the EPDiff equations. In particular, we illustrate the existence and dynamics of traveling wave solutions of the EPDiff equations. Solitary waves for this class of equations can be made to correspond to interacting particles of a finite-degree-of-freedom Hamiltonian system. We analyze the dynamics of two-solitary wave interaction and show that two solitons can either scatter or capture each other. The scattering or capture orbits depend on the singularity level of the solitons, while singularity of a soliton is determined by the power of the linear elliptic operator associated with the EPDiff equations.

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CP3

The Gaussian Semiclassical Soliton Ensemble

We study a particular family of perturbed initial data for the focusing nonlinear Schrödinger equation. This family of data arises naturally in the analysis of the zero-dispersion limit. However, the ellipticity of the associated modulation equations raises questions about the impact of even small perturbations of the data. Remarkably, our experiments show that the rate of convergence of the perturbed data to the true data is propagated to positive times including times after wave breaking.

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CP3

Phyllotaxis As a Pattern-Forming Front

Some of the most spectacular patterns in the natural world can be found on members of the plant kingdom. Furthermore, the regular configurations of organs on plants, collectively termed phyllotaxis, exhibit a remarkable predisposition for Fibonacci-like progressions. Starting from a biochemical and mechanical growth model, we derive a PDE similar to the classic Swift-Hohenberg equation and find that nearly every property of Fibonacci phyllotaxis can be explained as the propagation of a pushed pattern-forming front.

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CP4

Automatic Segmentation of Microscopy Images Based on the Starlet Wavelet Transform

We propose an automatic method based on starlet wavelets to perform the segmentation of photomicrographs. The proposed segmentation method is given applying starlets in an input image, resulting in L detail levels. First and second detail levels are ignored; then, third to last detail levels are summed. From the original image and its Ground Truth, Matthews Correlation Coefficient (MCC) is calculated for each level application. Therefore, the optimal segmentation level has the highest MCC.

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CP4

The Generalized Haar-Walsh Transform (GHWT) for Data Analysis on Graphs and Networks

We present a new multiscale transform for data on graphs and networks which is a generalization of the classical Haar and Walsh-Hadamard Transforms. Using a recursive partitioning of the graph, the transform generates an overcomplete dictionary of piecewise-constant orthonormal bases. We adapt the best-basis selection algorithm to this setting, allowing us to choose a basis most suitable for the task at hand. We conclude with some results from approximation and classification experiments.

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CP4

Alternating Direction Approximate Newton (ADAN) Method for Partially Parallel Imaging

ADAN method is developed for problems that arise in partially parallel magnetic resonance image reconstruction (PPI). The reconstruction amounts to solving a problem of the form $\min\{\phi(Bu)+1/2\|Au-f\|^2\}$, where u is the image. It is shown that ADAN converges to a solution of the image reconstruction problem without a line search. It performs at least as well as the recent variable stepsize Bregman operator splitting algorithm (BOSVS), which requires a line search and a suitable choice for many algorithm parameters.

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CP4

Topology and Numerical Analysis in Molecular Simulations

Topological changes are significant during molecular simulations. Our research focuses upon accurate display of these changes through dynamic visualizations to domain scientists. Most topological characteristics are formulated in terms of infinite precision, raising challenges within the approximations seen for graphics. Problems and partial solutions will be presented.

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CP4

Per-Class Pca-Src: Increased Flexibility and Specificity in Sparse Representation-Based Classification

Sparse Representation-based Classification (Wright, et al.) seeks the sparsest decomposition of test samples over the dictionary of training samples. This method assumes that the number of classes is large and test samples lie in the linear subspaces spanned by their class' training data. We propose a modification that builds class-specific dictionaries containing approximate bases to points on the class manifold using the "local PCA' technique of Singer, et al. We show our modifications improve performance.

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CP4

Synchrosqueezed Wave Packet Transforms and Diffeomorphism Based Spectral Analysis for 1D General Mode Decompositions

We develops new theory and algorithms for 1D general mode decompositions. First, we introduce the 1D synchrosqueezed wave packet transform (SSWPT) and prove its ability to estimate the instantaneous information of well-separated modes from their superposition. The SSWPT has a better resolution than the synchrosqueezed wavelet transform. Second, we present a new approach based on diffeomorphisms for the spectral analysis of general shape functions. These two methods lead to a framework for general mode decompositions.

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CP5

Two Mode Matrix of Urban Structure

We present an urban network that takes into account how streets and neighborhoods interact and influence each other. This two-mode urban structure presents another approach to analyze urban environments. We use GIS to construct a network map of an American city and then apply network analysis to evaluate how the network structure influences such features as traffic flow, density and housing considerations. Also, given the rise of African cities, where some are being completely designed and developed in lieu of developing organically, the results of this project will make recommendations for effective metropolitan growth structures.

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CP5

Classifying Contagion Dynamics on a Noisy Network Using Persistent Homology

A contagion can exhibit complicated dynamics on a network and its spread may be constrained by an underlying geometry. We embed nodes of a complex-contagion model on a manifold (e.g. $\mathbb{R}^2$). We study the extent that a contagion adheres to the underlying geometry with noisy non-geometric edges by embedding the nodes as points in a metric space and analyse the geometrical/topological properties. We leverage our results to obtain insight into nonlinear dimension reduction.

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CP5

On Continuous Time Bounded Confidence Opinion Dynamics with Multidimensional Opinions

In the bounded confidence opinion dynamics model, the opinion of each agent is only affected by other agents whose opinions lie within a confidence bound. In the case of continuous time bounded confidence opinion dynamics model with scalar opinions, trajectories have been proven to reach an equilibrium asymptotically in time. We generalize this result for vector opinions by introducing *Dissipation functions* and studying omega-limit sets of the trajectories.

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CP5

Numerical Study on G-Expectation

We will present some numerical methods for the G-Heat equation which is related to the nonlinear expectation, introduced by Shige Peng:

$$u_t - G(D^2u) = 0,\ (x,t) \in R^n \times (0,T);\quad u(x,0) = \phi(x),$$

where $G(A) = \sup_{Q\in\Theta}(\frac{1}{2}tr(AQ))$, $\Theta \subset S_+(n) = \{BB^t : B \in R^{n\times n}\}$ Numerous numerical experiments will be carried out to show the efficiency, accuracy and stability of the proposed methods. The effect of the boundary conditions is also numerically investigated. Some numerical analysis is given to show the convergence of the numerical solutions to the viscous solutions of the G-Heat equation.

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CP5

Support System for Mathematical Models Based on Optimization Problems of Economic Agents

This paper presents a support system for economic modeling. It supports development, numerical computations and analytical study of models. It also controls balances and dimensions of a model for correctness and consistency. It was successfully applied to intertemporal equilibrium models of the Russian and the Kazakhstan economies. The system is particularly efficient for structures similar to general economic equilibrium with nonstandard descriptions of agents. The system is supplemented by special procedures of regularization of complementary slackness conditions, subsystem for analysis of stationary (or more exactly self-similar) solutions, based on the dimensions of the system, as well as an algorithm for solving the model as a boundary value problem and its implementation on a supercomputer.

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CP6

Solution of a 2D Electrodiffusion Problem: Mathematical Modeling of Contact Resistance in Silicon Photovoltaic Cells

In screen-printed silicon-crystalline solar cells, the presence of a thin interfacial glass layer of varying thickness between the silicon and silver electrode inhibits electron flow. In this paper we analyze a model for electron transport across the glass, based on the 2D drift-diffusion equations. We solve the model numerically using a spectral method and compare results to asymptotic solutions. We are able to determine the effect of different glass layer topographies on the contact resistance.

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CP6

Eigenvalue Problems for Rapidly Growing Operators in Divergence Form

In an Orlicz-Sobolev setting, the spectrum of an exponential type perturbation of the Laplace operator is completely characterized by means of an asymptotic analysis of a class of eigenvalue problems involving the p-Laplacian. This talk is based on joint work with Mihai Mihăilescu (University of Craiova and "Simion Stoilow" Institute of Mathematics of the Romanian Academy, Bucharest, Romania).

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CP6

Simulating Non-Dilute Transport in Porous Media Using a TCAT-Based Model

Predicting the transport of non-dilute species in fluids of variable density in porous media is a challenging problem. We use a thermodynamically constrained averaging theory (TCAT)-based model, which consists of a flow equation, a species transport equation, and closure relations. We rewrite the model as a system of two partial differential-algebraic equations. We use a stiff temporal integrator to perform 1D simulations. The model is nonlinear and nonsmooth. We will discuss results and numerical difficulties.

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CP6

A General Methodology for Approximating the Discrete Chemical Master Equation with Short Range Spatial Correlations in Homogeneous Systems

The chemical master equation is used to describe a wide variety of chemical kinetic processes, however the resulting system is posed in an infinite dimensional space. Often, this system is solved via realizations of stochastic differential equations via kinetic Monte Carlo methods, however these techniques may have high computational cost and require statistical sampling over many realizations. In cases where the system of interest may be assumed to have short range spatial correlations and have translational symmetries, we demonstrate a general methodology of approximating the chemical master equation by a finite dimensional system of ordinary differential equations. We then demonstrate this methodology with a concrete example of surface catalysis and compare our results with those from kinetic Monte Carlo simulations.

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CP6

On the Initial-Boundary Value Problem for the Korteweg-De Vries Equation

The Korteweg-de Vries Equation (KdV Equation) is one of the most important nonlinear PDEs of applied mathematics. We will discuss the initial-boundary problem for the PDE and show, depending on boundary conditions, that it can behave like a hyperbolic PDE such as the wave equation and has time reversible solutions, and it can also behave like a parabolic equation such as the heat equation and has smooth solutions that are not time reversible.

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CP6

Transmission Eigenvalues for Regions on a Conducting Surface

We consider the interior transmission problem corresponding to inverse scattering for a bounded isotropic dielectric medium lying on an infinite conducting surface. In particular, we investigate the 2-D scalar case where the dielectric medium is illuminated by time harmonic Transverse-Electric or Transverse-Magnetic polarized electromagnetic waves. In both cases we show that transmission eigenvalues exist and form a discrete set. Numerical results are given showing that real transmission eigenvalues can be found from near field data.

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CP7

Robust Dynamic Shaping of Distributed Parameter Systems Via Recursively Updated Empirical Basis Functions

We focus on shaping the dynamic response of distributed parameter systems in the presence of parameter uncertainty using adaptive model order reduction. The problem is addressed by enforcing the desired spatio-temporal dynamics in the closed-loop system via an observer-based robust nonlinear feedback controller specifically designed based on the reduced order model that is refined by recursively updated empirical basis functions. The proposed method is illustrated on the thermal dynamic shaping in a catalytic reactor.

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CP7

Anytime A* for Continuous Optimal Path Planning

Eikonal PDE can be used to find the value function of an isotropic optimal control problem. These PDE can be solved efficiently using the Fast Marching Method, and A* methods provide additional computational savings. We present an Anytime algorithm using FMM and ideas from Weighted A*, quickly producing an initial suboptimal solution that is iteratively improved. This ensures early availability of a suboptimal path before the completion of the search for a globally optimal path.

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CP7

A Proper Orthogonal Decomposition Based Method for Solving Algebraic Riccati Equations

We present a new method to solve algebraic Riccati equations by employing a projection method based on Proper Orthogonal Decomposition. The method only requires simulations of linear systems to compute the solution of a Lyapunov equation. The leading singular vectors of the Lyapunov solution are then used to construct a projector which is employed to produce a reduced order system.Computational results and comparisons to other methods will be discussed.

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CP7

A New Semi-smooth Newton Multigrid Method for Parabolic PDE Optimal Control Problems

A new semi-smooth Newton (SSN) multigrid algorithm is proposed for solving the discretized first order necessary optimality systems that characterizing the optimal solutions of a class of 2D semi-linear parabolic PDE optimal control problems with control constraints. To achieve a second-order accurate finite difference discretization, we use a leapfrog scheme (with the second-order backward differentiation formula (BDF2)) in time and a standard 5-point stencil in space. The derived well-structured discretized Jacobian matrices greatly facilitate the development of effective smoother in our multigrid algorithm. Numerical simulations are provided to illustrate the efficiency of the proposed method, which validates the second-order accuracy in solution approximations and the optimal linear complexity in computational time.

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CP7

Computationally-Based Technique for Bifurcation Control

In this paper, a computationally-based methodology to obtain chaos controllers for PWM buck power converters is proposed, developed and proven. The mathematical model of a PWM is highly nonlinear (and non-smooth) and simulations show rich phenomena. The controller is easy to implement with an analog circuit, and it improves the performance of the system. Additionally, it reduces the percentage of regulation error and eliminates non-desired orbits. Computational and experimental results validate the controller design.

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CP8

Accelerated Hierarchical Stochastic Collocation - Finite Element Methods for PDEs with Random Inputs

The dominant cost of stochastic collocation methods for PDEs with high-dimensional random inputs are the cost of solving large numbers of linear systems. For non-intrusive methods like stochastic collocation, each linear system can be solved separately. Instead we consider global and local, hierarchical, semi-intrusive methods that accelerate the performance of the finite element solvers and look at the conditions under which computational costs can be reduced.

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CP8

Uncertainty Qualification Based on Ranking Fuzzy Numbers

In this paper, we present a new method for uncertainty qualification based on ranking fuzzy number. First, we present a new method for ranking fuzzy numbers. It considers left and right area deviation. The proposed method can overcome the drawback of some existing methods for ranking fuzzy numbers. Then, we apply the proposed method for ranking fuzzy numbers to develop a new method for dealing with fuzzy risk analysis problems.

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CP8

Reduced Basis Methods for Maxwell's Equations with Stochastic Coefficients

We consider parametrized partial differential equations in many-query settings. We discuss the Reduced Basis Method (RBM) for time-harmonic Maxwell's equations under stochastic parameters. The RBM model reduction significantly reduces the system size while preserving a certified accuracy by employing rigorous error estimators. To quantify the statistical outputs like mean and variance for Maxwell's equations under stochastic uncertainties, we use sparse collocation and weighted RBM. Numerical experiments are performed on 3D models of microwave devices.

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CP8

Use of Polynomials of Chaos as Regression Functions for Universal Kriging Models and Application to Numerical Dosimetry

In the computer experiments domain, Universal Kriging and Polynomial Chaos are two widely used metamodeling approaches. Considering a sparse representation of the Polynomial Chaos expansion gathering the most influent polynomials with the Least Angle Regression, this communication proposes to use these polynomials as regression functions in the Universal Kriging model. The optimal performances of the proposed approach are illustrated with several benchmark functions and with a dosimetry example.

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CP8

Quasi Optimal Sparse-Grid Approximations for El-

liptic PDEs with Stochastic Coefficients

Solution of PDEs depending on random coefficients can be conveniently approximated by polynomial expansions on the parameter space, that suffer however from a performance degradation as the number of random parameters increases ("curse of dimensionality' effect). In this talk we will propose an "a-priori/a-posteriori knapsack approach' to minimize such effect for sparse grids approximations. The efficiency of the proposed technique will be supported by theoretical convergence results and numerical tests.

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CP9

Subharmonic Response and Threshold of Chirp Driven Microbubbles

Recent experimental results have shown that acoustically driven microbubbles may exhibit an enhanced subharmonic response if driven by nonstationary (chirp) waveforms. However, the previous theory on the subharmonic threshold has been limited to single frequency forcing. We present a method for predication of the threshold using a energy ratio of the IMFs from a Empirical Mode Decomposition of the scattered acoustic signal. Results are compared for linear and finite elastic models of an encapsulating shell for ultrasound contrast agent microbubble applications.

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CP9

A Global Bifurcation of Mixed-Mode Oscillations

Mixed-mode oscillations (MMOs) are trajectories of dynamical systems in which large and small oscillations occur with a distinct gap between the two. Over two decades ago, Koper first observed the seemingly paradoxical emergence of complex MMOs in a (now canonical) model. We describe the successful detection of an elusive global bifurcation that only now resolves this paradoxical dynamics. Our techniques are based on computation of invariant manifolds and continuation methods.

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CP9

Mixing and Piecewise Isometries on a Hemisphere

We study chaotic nonlinear dynamics and mixing on a hemispherical surface using piecewise isometries (PWI) motivated by cutting and shuffling in 3-D granular flow. Mapping singularities with simple PWI for different parameters yield a variety of complex patterns on the hemisphere's surface termed the exceptional set (E). Coarse-grained measures of E suggest that E exhibits properties of fat fractals that may provide deeper insight into mixing by cutting and shuffling.

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CP9

Variational Integrators for Interconnected Dirac Mechanical Systems

Dirac mechanics simultaneously generalizes Lagrangian and Hamiltonian mechanics to reveal the geometric structure of systems with forces, constraints and degeneracies. Jacobs and Yoshimura recently elucidated the relationship between the Dirac mechanical structure of an interconnected system and those of its components. The variational integrator construction derives structure-preserving integrators from discrete variational principles, producing symplectic, momentum preserving integrators where applicable. This talk will discuss extensions of existing Dirac variational integrators to accommodate interconnections.

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CP9

Different Wave Solutions Associated with Singular Lines on Phase Plane

The bifurcation phenomena of a compound K(m,m) equation are investigated. Three singular lines have been found in the associated topological vector field, which may evolve in the phase trajectories of the system. The influence of parameters as well as the singular lines on the properties of the equilibrium points has been explored in details. Transition boundaries have been obtained to divide the parameter space into regions associated with different types of phase trajectories. The existence conditions and related

discussions for different traveling wave solutions have been presented in the end.

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CP10

A Domain Decomposition Method for Cavitation Computation in Nonlinear Elasticity

A domain decomposition method is applied to compute cavity growth in nonlinear elasticity. The idea is that the material is first tailored into nonoverlapping circular ring sub-domains so that each one is a scaling of the other; then, the standard Dirichlet to Neummann boundary conditions are applied to pass the information from a subproblem to its neighbors; finally, some special measures are taken to stabilize the method. The convergence speed is greatly improved by the method.

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CP10

On Strong Ellipticity for Implicit and Strain-Limiting Theories of Elasticity

Implicit constitutive theories for elastic material bodies have received increasing attention in the literature. The theories are used to formulate strain limiting models of elasticity, and to develop nonlinear constitutive relations between linearized strain and stress. We study strong ellipticity for a general class of elastic implicit constitutive relations and apply it to specific examples. For the considered examples, strong ellipticity is shown to hold for sufficiently small strain and fail for suitably large strain.

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CP10

Direct Numerical Simulation of Anti-Plane Shear Fracture in New Class of Elastic Bodies

In this work we study Finite Element Method (FEM) for the problem of anti-plane shear fracture in the setting of a strain-limiting theory of elasticity. Recently Rajagopal and Walton used a new class of such models to study anti-plane strain fracture. Using asymptotic analysis of the model near the tip of crack, they showed that both stress and strain vanish at the crack-tip, and the crack separation displacement has a cusp-shaped profile. The FEM based direct numerical simulation indicates that the present approach removes the classical square root singularity and hence predicts bounded stress and strain at the crack-tip.

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CP10

Peridynamics As a Multiscale Method

The peridynamic theory of solid mechanics is a strongly nonlocal theory that contains a length scale representing the maximum interaction distance between material points. Recent work shows that by varying this length scale, we can achieve a multiscale model of solids within a single theory, without the need to couple dissimilar methods. In this talk I will describe a hierarchical multiscale method based on the peridynamic equations and appropriate coarse graining of material properties.

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CP10

Light Beam Interaction in Nonlinear Optical Media

The dynamics of light beam interaction in Nonlinear Optical Media is studied numerically and analytically. The beam dynamics is simulated by the beam propagation method. The numerical results agree with the results of the analytic model. The results show that the reflection and transmission can be predicted and controlled by the trapped beam at the interface of two nonlinear optical media. Some interesting new results will be presented in this talk.

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CP11

Variance Reduction in the Simulation of Stochastic Differential Equations

Variance reduction techniques are commonly used to enhance the efficiency of Monte Carlo simulations. This talk focuses on variance reduction for single and coupled systems of stochastic ordinary differential equations. Variance reduction techniques such as antithetic variates and control variates will be described and results presented.

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CP11

A Guaranteed Automatic Integration Library for Monte Carlo Simulation

This talk introduce the Guaranteed Automatic Integration Library (GAIL), which was developed within last year. It

contains four algorithms, which perform function approximation, numerical integration(using Monte Carlo method and 1-D trapezoidal rule) and Monte Carlo for evaluating the mean. All routines come with theoretical guarantees of success, something that is missing, say, for MATLAB's `integral.m` and nearly all other automatic algorithms. Moreover, GAIL has been carefully designed with a friendly user-interface, thorough documentation, and extensive testing. Also, this talk discuss the theoretical research on the reliable relative error estimation based on the previous work, which comes with the numerical results and proved theorems.

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CP11

Reliable Error Estimation for Quasi-Monte Carlo Methods

This project aims to build an efficient algorithm based on extensible rank-1 lattice rules for multidimensional integration with guarantees. In order to proceed, we compute the a Fast Fourier Transform on the integrand values sampled on an integration lattice and use them to approximate the Fourier coefficients of the integrand. The decay rate of the Fourier coefficients and the assumption that the integrands lie inside a given cone helps us approximate the error.

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CP11

Split-Step Balanced Milstein Methods for Multi-Channel Stiff Stochastic Differential Systems

We discuss systems of ordinary SDEs with non-commutative multi-channel noise arising in chemical networks that involve reactions at different time scales. Such systems are inherently stiff, both in deterministic and stochastic components, and can change stiffness with uncertainty. To resolve this issue we consider fully implicit split-step balanced methods with optimal parameter selections with respect to the desired convergence, stability and positivity properties. Numerical examples are provided to show the effectiveness of these methods.

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CP11

Local Smoothers for Cdfem with Sub-Element Discontinuities

The conformal decomposition finite element method (a technique for handling sub-cell discontinuities) allows for Lagrangian-like interfaces in a (basically) Eulerian mesh. As the physics "chooses" the location of the interface, it can lie very close to element boundaries, which can hurt matrix conditioning and the linear solver. We present a local smoothing multigrid approach, which uses information about geometry near the interface to perform a single geometric coarsening to a problem with volume-averaged materials.

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CP11

Various Strategies for the Numerical Stochastic Homogenization of the Stochastic Poisson and Helmholtz Equations

We consider stochastic versions of the Poisson equation as well as of the Helmholtz equation with discontinuous coefficients. These equations arise, e.g., when modeling nanowire sensors and metamaterials with a random structure. Although there are some theoretic homogenization results, the question of how to compute solutions efficiently still remains. Here, we discuss approximations of the stochastic dimensions by various quasi-MC strategies and which boundary conditions and size of the domain to use when approximating the problem on the whole space.

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CP12

Iron-dependent Oxidative Stress Response Pathway in Human Mammary Epithelial Cells

It has been known that iron plays an important role in the development of breast cancer and cancer cells are under persistent oxidative stress. However, the effect of iron overload on the oxidative stress response pathway in normal and cancer cells is still under study. This project focuses on a mathematical model of an oxidative stress response pathway in normal human breast cells in order to understand how normal cells transition malignant cells.

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CP12

A Mathematical Model for Glucose and Fatty Acid Metabolism

A model is presented for the rate of utilization and storage of carbohydrates and fats. It is based on differential equations for the chemical kinetics converting glucose and fatty acids to pyruvate and acetylCoA, which then enter the Krebs cycle to produce energy. The molecules can also be stored as glycogen and fat. The conversion rates are modeled as Hill's reactions. Results are presented for different conditions of supply and usage.

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CP12

Multiscale Simulation of Reaction-Diffusion Systems in Living Cells

We present a simulation algorithm that allows for dynamic switching between a microscopic and a mesoscopic modeling framework for stochastic reaction-diffusion kinetics. By discretizing space with an unstructured mesh we can carry out simulations in complex and realistic geometries. The accuracy and efficiency of the algorithm is demonstrated in numerical examples inspired by biological applications. We show that by simulating only parts of a system at the more detailed, microscopic level, we can reduce the computational cost significantly while retaining the accuracy of the full microscopic model. The method can be combined with microscopic simulations of dynamic lower dimensional structures such as DNA or fibers, where the microscopic simulations are used close to the complex parts of the geometry, and the more efficient mesoscopic simulations are used in the other parts of space.

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CP12

A Simulator of the Multi-Scale Dynamics of Gene Regulatory Networks

We propose a simulator of an ODE model class of the multiscale dynamics of gene regulatory networks with steep sigmoidal interactions. The threshold-dependent dynamics divides the phase space into domains. Under specific assumptions, trajectories through any sequence of domains are derived by iterating a local computation of transitions between domains. The parameter values can be expressed either qualitatively by inequalities or by probability distribution. In the latter case, the probability of trajectory occurrence is calculated.

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CP12

Bioechemical Network Structure can be Revealed with Timecourse Data

Due to the limit of current experimental techniques, identifying biochemical network among genes and proteins underlying biological systems is one of the most challenging works. On the other hand, output of the networks, timecourses of genes and proteins can be easily acquired with recent advances in technology (e.g. microarray analysis). In this work, we will describe how to use oscillating timecourse data to reveal the biochemical network structure by using a fixed-point criteria.

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CP12

Using Machine Learning and Metabolomic/transportomic Systems Modeling to Identify Bacterial Ecotype from Genomic Sequence of Uncharacterized Environmental Or Clinical Isolates

The ability to genomically sequence bacteria from environmental or clinical isolates that are not or cannot be cultured in the laboratory requires development of computational tools to predict bacterial ecotypes from genomic data. Using Psuedomonads for which complete genomes are available and ecotype is known or inferred, we demonstrate that support vector machines using features derived from computational modeling of bacterial metabolome and transportome is more predictive of Psuedomonads ecotype than using only genomic data.

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CP13

Non-Parametric Clustering with Rank-Constrained Least-Squares

Unsupervised clustering is a problem of great practical importance, from genetics to marketing, extreme events modelling or even financial engineering. Although most available techniques perform well in practice, most of them require solving an NP-hard optimization problem or require to know the number of clusters ahead of time. Our goal is to present a simple technique for fast joint estimation of the number of clusters and their respective center of mass. Assuming the data can be represented as a $d \times n$ matrix $X = C + E$, where $C = MT$, E is a matrix-noise, M is the center of mass matrix, and $T_{k,i} = 1$ if X_i belongs to custer k and $T_{k,i} = 0$ otherwise. This representation leads to searching for a low rank approximation of X. The rank of C is the number of clusters and is efficiently estimated using recent work in model selection. The approximation itself can be performed using the power method and its recent analysis by Hardt.

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CP13

Stationary Stability for Evolutionary Dynamics in Finite Populations

We extend the theory of evolutionary stability to multidimensional finite populations with mutation, connecting the theory of the stationary distribution of the Moran process with the Lyapunov theory of evolutionary stability for the replicator dynamic. We show essentially that the local extrema of the stationary distribution minimize the relative entropy of the current population state and the "expected next state" computed by weighting the adjacent states by the appropriate transition probabilities. This holds for a variety of selection processes including the increasingly popular Fermi selection. We present several complete computational examples for illustration and we show that the classical stability theory of the replicator dynamic is recovered in the large population limit. If time allows, we describe extensions to populations evolving on graphs.

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CP13

A Novel Concept of Normal Exponential ROC Model

Receiver Operating Characteristic (ROC) Curve is used to quantify and compare the accuracy of diagnostic tests. In this paper, Normal Exponential ROC model is proposed and its properties are studied when healthy test scores follow Normal distribution and diseased test scores follow Exponential distribution. Area under the proposed ROC curve and its standard error are derived. The utility of this model is explored using simulation studies and Serum concentrations of CA 19-9 (Carbohydrate antigen) for pancreatic cancer. At the end, it is found that proposed ROC model gives better accuracy as compared to the traditional Binormal ROC model.

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CP13

Storage Allocation Models with Finite Capacity

We consider a stochastic storage allocation model, which has m primary holding spaces and R secondary ones. All of the spaces are numbered and ordered, and an arriving customer takes the lowest ranked available space. We define the traffic intensity ρ to be λ/μ where λ is the customers' arrival rate and μ is the service rate of the processor. If we let $m+R=N$, the total number of stored items behaves as an $M/M/N/N$ queue, which is the Erlang loss model. We obtain the joint probability distribution of the numbers of occupied primary and secondary spaces, for $\rho \to \infty$. We also study the marginal distribution of the number of occupied secondary spaces, as well as various conditional distributions.

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CP14

Using Lasso Model to Predict Cell-Type-Specific Transcription Factors in Low Methylated Regions

Low Methylated Regions (LMRs) have been implied to be potential distal regulatory regions. Using the transcription factor binding sites (TFBSs) predicted from both LMRs and promoters, we apply LASSO models to predict directions of gene expression among multiple cell types based on the similarity score of TFBSs. By analyzing the LASSO results, we demonstrate that the model can facilitate the identification of cell-type-specific transcription factors binding that may potentially regulate directions of gene expression.

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CP14

Moment Fitting for Parameter Inference in Repeatedly and Partially Observed Stochastic Biological Models

The inference of reaction rate parameters in biochemical network models from time series concentration data is a central task in computational systems biology. Under the assumption of well mixed conditions the network dynamics are typically described by the chemical master equation. Based on the latter we derive closed systems of parameter dependent nonlinear ordinary differential equations that predict the time evolution of the statistical moments. For inferring the reaction rate parameters we suggest to not only compare the sample mean with the theoretical mean prediction but also to take the residual of higher order moments explicitly into account. Cost functions that involve residuals of higher order moments may form landscapes in the parameter space that have more pronounced curvatures at the minimizer and hence may weaken or even overcome parameter sloppiness and uncertainty.

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CP14

Mathematical Modeling of the Antibiotic Er-

tapenem

Ertapenem is an antibiotic commonly used to treat a broad spectrum of infections. A physiologically-based pharmacokinetic model was developed to investigate the uptake, distribution, and elimination of ertapenem following a once-a-day, single one gram dose. Blood concentrations of ertapenem found by the model were compared to data from published experimentation for normal height, normal weight males. Simulations were performed to consider the distribution of the antibiotic in underweight, overweight, and obese men of normal height.

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CP14

Connecting Motifs and Molecular Mechanisms Toward Control of Complex Networks

Advances in high throughput biological assays have promoted statistical inference of large experimental datasets; the subsequent networks are then used as models to discover therapeutic targets. However, these networks yield little mechanistic insight into the cornerstones of complex biological systems: regulation and dynamics. Comprehensive analysis of networks inferred from *in silico* models that represent biological mechanisms (*e.g.*, competitive inhibition) elucidates our understanding of large network dynamics and informs novel control strategies.

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CP14

A Combined Method of Model Reduction for Biochemical Reaction Networks

This talk introduces a combined model reduction algorithm with particular application to biochemical reaction networks within the context of systems pharmacology. This method brings together versions of proper lumping and empirical balanced truncation to reduce nonlinear, stiff dynamical systems that are typical in the modelling of biochemical reactions. Modifications and enhancements to the established methods are discussed. Finally, the algorithm is demonstrated with application to two published systems biology models, with good results.

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CP14

Discovery of Multi-Dimensional Modules in Cancer Genomic Data

Recent technology has made it possible to simultaneously perform multi-platform genomic profiling of biological samples, resulting in so-called 'multi-dimensional genomic data'. However, integrative analysis of multi-dimensional genomics data for the discovery of combinatorial patterns is currently lacking. Here, we develop a set of matrix factorization techniques to address this challenge. We applied this method to the data from the The Cancer Genome Atlas project, and show that our tools can uncover hidden patterns in multi-dimensional cancer 'omic' data.

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CP15

Fourth Order Compact Simulation of the One Dimensional Euler Equations of Gas Dynamics

This paper introduces a class of higher order compact schemes for the solution of one dimensional (1-D) Euler equations of Gas Dynamics. These schemes are fourth order accurate in space and second or lower order accurate in time and unconditionally stable. To test the efficiency of our proposed schemes, we first apply it to three shock tube problem of gas dynamics, including the famous SOD shock tube problem. Later on, we apply our proposed schemes to the subsonic-supersonic isentropic flow through a convergent-divergent nozzle and compare our solution with the exact solutions. In all the cases, our computed numerical solutions are found to be in excellent match with the exact ones. Lastly, we show ways to extend the schemes to problems of higher spatial dimensions.

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CP15

High Order Parametrized Maximum-Principle-Preserving and Positivity-Preserving Weno Schemes on Unstructured Meshes

We will talk about the generalization of the maximum-principle-preserving (MPP) flux limiting technique developed in [Z. Xu, Math. Comp., (2013)] to develop a class high order MPP finite volume schemes for scalar conservation laws and positivity-preserving (PP) finite volume WENO schemes for compressible Euler system on two dimensional unstructured meshes. The key idea of this parameterized technique is to limit the high order schemes towards first order ones which enjoy MPP property, by decoupling linear constraints on numerical fluxes. Error analysis on one dimensional non-uniform meshes is presented to show the proposed MPP schemes can maintain high order of accuracy. Similar approach is applied to solve compressible Euler systems to obtain high order positivity-preserving schemes. Numerical examples coupled with third order Runge-Kutta time integrator are reported.

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CP15

Scalable High-Order Non Conforming Finite Element Methods For Time Domain Acoustic-Elastic Problems

High-order numerical methods for solving time-dependent acoustic-elastic coupled problems are introduced. These methods, based on Discontinuous Galerkin and Classical Finite Element techniques, allow for a flexible coupling between the fluid and the solid domain by using non-conforming meshes and curved elements. Importantly, physical domains may be independently discretized and the structural geometry is faithfully represented upon a chosen degree of fidelity, enabling for higher flexibility and efficient computation. In order to illustrate the accuracy and scalability properties of a parallel implementation, we present representative numerical tests for large-scale seismic wave propagation.

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CP15

Advances in Adaptively Weighted Finite Element Methods

The overall effectiveness of finite element methods may be limited by solutions that lack smoothness on a relatively small subset of the domain. By enhancing norms and and/or inner products in the variational framework with weight functions chosen according to a coarse-scale approximation, it is possible to recover near-optimal convergence rates. In this talk we give an overview of the general approach, both in the least-squares and Galerkin settings, and illustrate with numerical examples.

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CP15

Numerical Simulations of Bioresorbable Vascular Stent with Automatic Patient-Specific Geometry Construction and Adaptive Meshing

The invention of Bioresorbable Vascular Stent(BVS) opened a new era for cardiovascular intervention technology as it offers numerous benefits for patients. Patient-specific CFD Simulation of stented vessel is a great tool to analyze potential risks of BVS such as restenosis. Current work in BVS research is limited to geometries with no clear appearance of the stent. However, we have developed an algorithm that extracts the 3D geometry of the deployed stent from real patients OCT images. Visualization of the blood flow in stented vessel for the first time becomes a reality. Combined with an adaptive meshing method, real inflow, and real vessel curvature, our CFD simulations can best approximate the real hemodynamic conditions of the stented vessel and provide many desirable results, which demonstrates the great power of numerical PDEs in biomedical engineering.

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CP15

A Finite Element Method for the Second Order Linear Elliptic Equation in Non-Divergence Form

We design a finite element method for the linear elliptic equation in non-divergence form, which satisfies discrete maximum principle. We show that the method guarantees convergence to the viscosity solution provided that coefficient matrix $A(x)$ and function $f(x)$ are continuous. In order to establish a rate of convergence, we derive a discrete version of Alexandroff-Bakelman-Pucci estimate. Using this discrete estimate, we show that

$$\| u - u_h \|_{L^\infty} \leq C \left(h^2 \ln \frac{1}{h} \right)^{\alpha/(2+\alpha)}$$

for $u \in C^{2,\alpha}(\Omega)$, $f \in C^\alpha(\Omega)$, and

$$\| u - u_h \|_{L^\infty} \leq C \left(\ln h^2 \frac{1}{h} \right)^{1/2}$$

for $u \in C^{3,1}(\Omega)$, $f \in C^{0,1}(\Omega)$.

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CP16

The Influence of Stochastic Parameters on Calcium Waves in a Heart Cell

In this study, we investigate the effects of stochastic release from calcium release units (CRUs) on generating calcium waves considering a distribution for the flux density term sampled (i) once for all CRUs and (ii) for each CRU independently. We include a stochastic flux density term as more physiologically appropriate than a fixed release rate. We use an array of statistical techniques as well as parallel computing to facilitate the large number of simulation runs.

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CP16

Simulation of Calcium Waves in a Heart Cell on Modern Parallel Architectures

Simulating calcium induced calcium flow in a heart cell requires solving a system of advection-reaction-diffusion equations in three space dimensions. Efficient parallel computing is necessary to enable long-time simulations on high-resolution meshes. Modern architectures with multiple memory hierarchies in CPU and coprocessors such as GPUs and the Intel Phi offer opportunities to speed up the numerical kernels of PDE solvers dramatically.

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CP16

A Model of Brain Neuro-Mechanics

Brain tissue is sensitive to mechanical forces and chemical imbalances which can alter brains functions and/or structure and lead to neurological diseases. Mathematical models of brain neuro-mechanics can increase our understanding of how brain works and help develop better diagnostic and therapeutic tools. We propose to model the brain as a mixture material and investigate the linkages between neural activity and mechanical behavior of brain tissue through computer simulations.

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CP16

Stochastic Homogenization of the One-Dimensional Keller-Segel Chemotaxis System

In this talk, we focus on the one-dimensional Keller-Segel chemotaxis system in a random heterogeneous domain. We assume that the corresponding diffusion and chemotaxis coefficients are given by stationary ergodic processes, and we apply methods pertaining to stochastic two-scale convergence to derive the homogenized macroscopic equations. Special attention is paid to developing numerical algorithms for approximating the homogenized asymptotic coefficients. This is joint work with Mariya Ptashnyk.

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CP16

Neural Implementation of Shape-Invariant Touch Counter Based on Euler Calculus

One goal of neuromorphic engineering is to imitate the brain's ability to count the number of objects based on the global consistency of the information from the population of visual or tactile sensory neurons whatever the objects' shapes are. To achieve this flexibility, it is essential to utilize topological methods rather than ad hoc algorithms. Although latest works by mathematicians tackled fundamental problems for shape-invariant count, they lack the circuit implementations to save computational time for big data. Here we propose a fully parallelized algorithm for a shape-invariant touch counter for 2D pixels. The touch number is counted by the Euler integral, a generalized integral, in which a connected component counter for binary images (Betti number) was used as elemental module. Through examples, we demonstrate how the proposed circuit embodies the Euler integral in the form of recursive vector operations, with scalability to high resolutions of pixels.

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CP17

Interface Tracking Using Level Set and A Fast Algorithm

Although moving interface problem is an interesting problem in physics, it is challenging to obtain accurate and stable numerical solution because interface problems are singular and sensitive with small perturbations. In this talk, we will discuss an interface tracking method for the solution of 2D incompressible Stokes flow problems within an unit disk as an application of a fast algorithm [L. Borges and

P. Daripa, *A fast parallel algorithm for the Poisson equation on a disk*, J. Comput. Phys., 16 (2001), pp. 151–192.] which is based on the principle of convolution of integrals involving Green's function and exact analysis.

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CP17

Field-split Preconditioned Inexact Newton Algorithms

To improve the convergence of systems with unbalanced nonlinearities, the field-split preconditioned inexact Newton (FSPIN) algorithm is introduced as a complementary form of the additive Schwarz preconditioned inexact Newton (ASPIN) algorithm, based on partitioning of degrees of freedom in a nonlinear system by field type rather than by subdomain. We introduce two types of FSPIN algorithms: Jacobi-type and Gauss-Seidel-type, and we augment the classical Jacobi-type convergence theory for the latter.

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CP17

A Dual Iterative Substructuring Method with An Optimized Penalty Parameter

In this talk, we will present a domain decomposition method based on augmented Lagrangian. The proposed method imposes the continuity on the interface not only by using Lagrange multipliers but also by adding a penalty term which consists of a positive penalty parameter and a measure of the jump across the interface. The study for the proposed method with an optimized penalty parameter will be discussed in terms of its convergence analysis and practical efficiency.

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CP17

Redefining a Mimetic Curl Operator Using Gauss' Theorem with Applications in Computational Climate and Weather Modeling

The common way to define a Curl operator considers Stoke's Theorem and the concept of circulation. Common numerical discretizations for this operator also use this approach. In this work, we present a redefinition of the Curl operator using Gauss' Theorem instead. This redefinition allows us to present a discretization framework that naturally inherits all the desirable properties of the mimetic differential operators. We present the mathematical justification for this redefinition and we implement this mimetic Curl operator testing it on 2 and 3D test cases. Physical applications concern the computational study of hurricanes.

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CP17

Fast Structured Direct Spectral Methods for Differential Equations with Variable Coefficients

We study the rank structures of the matrices in Fourier- and Chebyshev-spectral methods for differential equations with variable coefficients in one dimension. We show analytically that these matrices have a so-called low-rank property, and develop a matrix-free direct spectral solver, which has nearly $O(N)$ complexity and $O(N)$ memory. Numerical tests for several important but notoriously difficult problems show the superior efficiency and accuracy of the direct solutions, especially when iterative methods have severe difficulties in the convergence.

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CP17

A Hybrid Fd-Fv Method for First-Order Hyperbolic Systems

We describe a hybrid FD-FV approach to solve first-order hyperbolic systems. These methods use cell averages and nodal values as dependent variables, and evolve them in time by the method of lines. They use the integral form of the PDE and Hermite interpolation polynomials to discretize the cell averages and nodal values in space, respectively. We present the accuracy and stability analysis of these methods to solve problems in one and two dimensions.

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CP18

Block Preconditioners for Biot's Equations

Biot's equations are a popular model for geomechanical simulations of fluid flow in elastic porous media. These simulations are run on a very large scale, resulting in a large number of unknowns. Further complicating matters is that the domains have complex geometry and a vast range of material parameters. The linear systems that arise after discretization of Biot's equations are large enough that iterative methods are required. They are also badly conditioned, making effective preconditioners essential. In this work we investigate the effectiveness of several different preconditioners over a wide range of material parameters.

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CP18

A Model for Tempo Synchronization in Music Performance

A model is derived for the manner in which performers of music establish and maintain tempi in the presence of a conductor, other performers, and noise. The model assumes that a performer sets a tempo in response to several stimuli. This tempo, or period, correction, occurs as a superposition of responses of the form of sensitivity times stimulus. The model is solved and results obtained for several cases. A model for phase correction is also derived.

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CP18

Recycling and Updating Preconditioners for Sequences of Linear Systems

For sequences of related linear systems, the computation of a preconditioner for every system can be expensive. Often a fixed preconditioner is used, but this may not be effective as the matrix changes. We analyze cheap updates to preconditioners: Incremental updates (Calgaro et al) and sparse approximate inverse updates to ILUTP preconditioners and updates to factorized sparse approximate inverse preconditioners (Bellavia et al.) Applications include model reduction, the Quantum Monte Carlo method, and others.

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CP18

Sensitivity of Leverage Scores to Perturbations

The leverage scores of a matrix A with full column rank are the squared row norms of any matrix that contains an orthonormal basis for the range of A. Leverage scores describe the importance of rows in regression problems and are used as sampling probabilities in randomized algorithms for matrix computations. We bound the difference between the leverage scores of A and a perturbation $A + \Delta A$ when the orthonormal basis is computed by a QR factorization or SVD.

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CP18

Symmetric Tensor Decompositions

A tensor is a multi-way or n-way array. A tensor is symmetric if its entries are invariant to any permutation of its indices. A tensor may also be symmetric with respect to a subset of its modes, i.e., if its entries are invariant to any permutation of a specific subset of its modes. We survey the landscape of symmetric tensor decompositions and compare various methods.

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CP18

Indefinite Preconditioning of the Coupled Stokes-Darcy System

We propose the use of an indefinite (constraint) preconditioner for the iterative solution of the linear system arising from the finite element discretization of coupled Stokes-Darcy flow. We provide spectral bounds for the preconditioned system which are independent of the underlying mesh size. We present numerical results showing that the indefinite preconditioner outperforms both standard block diagonal and block triangular preconditioners both with respect to iteration count and CPU times.

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CP19

Optimisation and Conditioning in Variational Data Assimilation

Data assimilation merges observations with a dynamical model to find the optimal state estimate of a system given a set of observations. It is cyclic in that it is applied at fixed time intervals and the beginning of each cycle incorporates the previous cycle known as the background or apriori estimate. Variational data assimilation aims to minimise a non-linear, least-squares objective function that is constrained by the flow of the (perfect) dynamical model (4DVAR).Relaxing the perfect model assumption gives rise to weak-constraint 4DVAR, which has two formulations of interest. Gradient-based iterative solvers are used to solve the problem. We gain insight into accuracy and convergence by studying the condition number of the Hessian. Bounds on the condition number are demonstrated using a simple model and are utilised to illustrate the effect of different assimilation components on the conditioning which can highlight interesting architectural differences between both formulations.

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CP19

A Primal-Dual Simplex Algorithm to Enumerate the Mixed Cells of a Polynomial System

When the polyhedral homotopy continuation method is used to locate all isolated zeros of a polynomial system, the process of enumerating all the mixed cells plays a critical role: it provides starting points for the solution paths and governs the efficiency of the continuation method. When locating mixed cells, one must deal with a large number of linear programming problems. Rather than the more popular interior point method, the simplex method is used for those LP problems because its underlying pivoting structure provides indispensable information in the process. An efficient primal-dual algorithm to enumerate all the mixed cells will be presented.

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CP19

Fitting a Straight Line in Three-Dimensional Space by Total Least-Squares Adjustment

Over a century ago Pearson (1901) solved the problem of fitting lines in 2-space to points with noisy coordinates in all dimensions. Surprisingly, however, the case of fitting lines in 3-space has seen little attention. We solve this problem using a new algorithm for the Total Least-Squares solution within an Errors-In-Variables (EIV) Model, respectively an equivalent Gauss-Helmert Model. Following Roberts (1988), only four parameters are estimated, thereby avoiding over-parameterization that may lead to unnecessary singularities.

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CP19

A Block-Coordinate Descent Approach for Large-Scale Sparse Inverse Covariance Estimation

The Sparse Inverse Covariance Estimation problem arises in many statistical applications in Machine Learning. In this problem, the inverse of a covariance matrix of a multivariate normal distribution is estimated, assuming that it is sparse. An l-1 regularized log-determinant optimization problem is solved to compute such matrices. Because of memory limitations, most algorithms are unable to handle large scale instances of this problem. We present a new block-coordinate descent approach for solving the problem for such large-scale data sets. Our method treats the sought matrix block-by-block using quadratic approximations. Numerical experiments demonstrate the potential of this approach.

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CP19

Coupled Spring Forced Multiagent Coordination Optimization for Mixed-Binary Nonlinear Programming

Mixed-binary nonlinear programming(MBNP) optimizing the network structure and network parameters simultaneously has been seen widely applications in cyber-physical system nowadays. Swarm intelligence based optimization algorithms simulate the cooperation and interaction behaviors from social or nature phenomena as optimization to solve complex, non-convex and/or ill-conditioned nonlinear problems of high efficiency. In this research, we propose a coupled spring forced multiagent coordination optimization (CSFMCO) algorithm by considering that each particle is a spring and is coupled with the optimal solution founded so far as the second abstract spring to offer a new efficient algorithm to solve the MBNP problem. Continuous optimizer, binary optimizer and the switch between

continuous and binary optimizers will be investigated.

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CP20

Modeling Accidental Explosions and Detonations

The physical mechanism and constraints required for a Deflagration to Detonation Transition (DDT) in a large number of explosive devices is investigated. The Uintah Computational Framework is utilized to model explosives using large computational platforms. Current efforts are focused on a parametric study to determine if inertial confinement could cause a transition to detonation. These simulations will give insight into the physical mechanism of DDT for large-scale explosions and help determine safe packaging configurations to eliminate DDT in transportation accidents.

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CP20

Finite Elements in Flux Coordinates in Gyrokinetic Turbulence Simulation

A series of finite elements with C^0 and C^1 continuity are constructed in curved flux coordinates in gyrokinetic turbulence modeling. The difficulties with flux coordinate Jacobian and periodic domain and the solution strategies will be demonstrated. This is the first time two-dimensional finite elements are constructed in this type of coordinate systems which are used everywhere in fusion plasma simulation.

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CP20

A Performance-Portable Implementation of the Albany Ice Sheet Model: Kokkos Approach

Modern HPC applications need to be run on many different platforms and performance portability has become a critical issue: parallel code needs to be executed correctly and performant despite variation in the architecture, operating system and software libraries. In this talk we'll present our progress towards a performance portable implementation of the finite element assembly in the Albany Ice Sheet Model code, based on Kokkos programming model from Trilinos.

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CP20

Matrix-Free Krylov Subspace Methods on Modern CPUs and Many-Core Processors

We study methods to implement Krylov Subspace methods in matrix-free form that take advantage of the memory hierarchy of modern CPUs and many-core processors such as GPUs and the Intel Phi. We also work to develop an effective preconditioner for Krylov subspace methods for linear systems arising from the discretization of PDEs that is easy to program. We use a finite difference approximation of an elliptic test problem for the computational experiments.

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CP20

Parallel Techniques for the Incomplete-LU Factorization

The incomplete-LU factorization (ILU) is one of the most popular black-box preconditioning techniques. However, incomplete factorizations are challenging to effectively implement on massively parallel computer architectures, such as GPUs. In this talk we present an in-depth study of different existing parallelization techniques for ILU, such as level-scheduling, multi-coloring and multi-level approaches, as well as more recent communication avoiding algorithms and related power(q)-pattern method. We discuss their properties and relationships. Finally, we present relevant numerical experiments.

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CP20

Effective Parallel Preconditioners for CFL Application

We focus on the fast iterative solution of linear systems on GPUs, in particular, for problems from computational fluid dynamics. Krylov subspace solvers mostly can be implemented efficiently on GPUs; however, the preconditioner is often a bottleneck. In fact, many of the most effective preconditioners perform poorly on GPUs, such as ILUT, taking much more time than the matrix-vector product in spite of similar complexity. Therefore, we discuss preconditioners like sparse approximate inverse preconditioners, which are matrix-vector product like, as alternatives, possibly accelerated with deflation techniques like Krylov subspace recycling.

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CP21

Equilibrium and Bifurcation Analysis of Discoidal Lipoproteins

A discoidal lipoprotein particle consists of a lipid bilayer bounded by a protein polymer chain. In isolation, the free energy of such a particle is the sum of the bending-energy of the bilayer and the bending and torsional energy of the chiral protein loop. The Euler–Lagrange equations governing the equilibrium of such particles are derived. Also, a finite-element solver is employed to obtain approximate numerical solutions and analyze possible conformations of these particles.

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CP21

Swimming and Pumping of Helical Bodies in Viscous Fluids

Many flagellated microorganisms including E. coli swim by rotating slender helical flagella, while ciliated organisms like Paramecia swim by passing helical waves along their surfaces. We will discuss a framework for studying such problems where the Stokes equations describing viscous flow are written in helical coordinates. Analytical predictions match well with full numerical simulations, and suggest optimal geometries. This work may also aid designs in microfluidic manipulation, microswimmer engineering, and the mixing of viscous fluids.

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CP21

Mathematical Model and Simulation of Particle Flow Around Choanoflagellates Using the Method of Regularized Stokeslets

Choanoflagellates are unicellular organisms whose intriguing morphology includes a set of collars/microvilli emanating from the cell body, surrounding the beating flagellum. We investigate the role of the microvilli in the feeding and swimming behavior of the organism using the method of regularized Stokeslets. This model allows us to depict the effective capture of nutritional particles and bacteria in the fluid and the hydrodynamic cooperation between the cell, flagellum, and microvilli of the organism.

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CP21

Swimming Efficiently: An Analytical Demonstration of Optimal Strouhal Number in Fish

Using Lighthills large amplitude elongated body theory it is shown that the kinematics of fish swimming can be reduced to a single variable, Strouhal Number (St). This is accomplished by applying mathematical constraints to enforce constant velocity, low drag swimming. Using this result, it is demonstrated that Froude efficiency for swimming can be defined directly as a function of St. This function correctly predicts the behavior of swimmers across a wide range of sizes.

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CP22

Analysis of a Large Time Step and Overlapping Grids Method for Hyperbolic Conservation Laws

We propose a numerical method for approximate solving of hyperbolic conservation laws. The method is based on a finite volume method and our novelties are twofold. First, our method is a Large Time Step method which enables us to march faster in time. Secondly, the method incorporates overlapping grids which is a very important issue in many practical applications. In one space dimension, we prove that the method converges to the entropy solution of the conservation law. We also present numerical simulations for Burger's equation and the Lax problem for the Euler gas dynamics equations.

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CP22

Filtered Positive P_N Closure for Kinetic Transport Equations

We propose a modification to the standard spherical harmonic closure, known as P_N closure, used for linear kinetic equations. The modification produces smooth, nonnegative polynomial particle distributions by using two-step filtering on the oscillatory, partially negative P_N solutions; closes the moment system using filtered polynomial ansatz; and integrates the closed moment system with filtered moments. We formulate the filtering process as a quadratic program, and demonstrate numerical results on the challenging line source benchmark problem.

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CP22

Unconditionally Optimal Error Estimates of Fully Discrete Fems for Parabolic Equations

Error analysis of fully discrete finite element methods for nonlinear parabolic equations often requires certain time-step size conditions (or stability conditions) such as $\Delta t = O(h^k)$, which are widely used in the analysis of the nonlinear PDEs from mathematical physic. In this talk, we suggest a new approach to analyze the discretization error of fully discrete FEMs for nonlinear parabolic equations. By this new approach, we found that the time-step size restrictions are not necessary for most problems. To illustrate our idea, we analyze some models from mathematical physics, e.g. the thermistor problem, miscible flow in porous media and gradient flows, with linearized backward Euler scheme for the time discretization. Previous works on the these models all required certain time-step size conditions.

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CP22

Asymptotic-Preserving Semi-Lagrangian Discontinuous Galerkin Schemes for a Class of Relaxation Systems

We consider in this work a class of singularly perturbed hyperbolic balance laws that admit a diffusive limit. Such systems arise naturally in radiative transport applications if one starts with a Boltzmann description and expands the distribution function in spherical harmonics (i.e., the Pn approximation). One key difficulty in solving such systems is that standard numerical schemes have maximum time-step restrictions that vanish in the singular limit. Several approaches have been proposed in the literature that overcome this difficulty, many of which are based on splitting the equation into stiff and non-stiff pieces and using appropriate semi-implicit time-stepping methods. In this work we employ a different strategy in order to achieve asymptotic-preservation. We develop a scheme using a discontinuous Galerkin semi-Lagrangian scheme. Several numerical test cases are used to validate the proposed scheme.

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CP22

Positivity-Preserving WENO Schemes with Constrained Transport for Ideal MHD

We will discuss a novel positivity-preserving flux limiting technique developed for WENO schemes to solve idea magnetohydrodynamic (MHD) equations. There are two main steps in our MHD solver: first updating conservative quantities by WENO scheme with positivity-preserving limiter and then correcting the magnetic field and total energy by a high-order constrained transport approach. Several examples are presented to verify the order of accuracy and to demonstrate the efficiency of positivity-preserving limiter.

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CP22

Partially Penalized Immersed Finite Element Methods for Elliptic Interface Problems

In this talk, we present new immersed finite element (IFE) methods for the second order elliptic interface problems on Cartesian meshes. Closely related to traditional IFE methods which are based on Galerkin formulation, these new IFE methods contain extra stabilizing terms at interface edges to penalize the discontinuity in IFE functions. Error estimation shows that these IFE methods converge optimally in an energy norm. Numerical examples demonstrate that these new methods outperform traditional IFE methods at the vicinity of the interface.

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CP23

Lagrangian Particle Methods for Global Atmo-

spheric Flow

We present a particle method for global atmospheric flow in spherical geometry based on the Lagrangian formulation of the fluid equations. Poisson equations for the stream function and velocity are solved using integral convolution with Green's function for the sphere, which is approximated numerically with singular point vortices and point sources using midpoint rule quadrature. An adaptive remeshing procedure is applied at regular time intervals to maintain spatial accuracy on the Lagrangian particles. Solutions of the barotropic vorticity equation are presented, and ongoing work with the shallow water equations is discussed.

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CP23

Numerical Derivation of a $\dot{D}-D-\kappa$ Relation for An Expanding Detonation Wave in the Mie-Gruneisen Equation of State

The propagation behavior of a detonation wave expansion can be described asymptotically by Taylor blast wave theory (TBW) in the limit of a small, rapid wave, and by geometrical shock dynamics (GSD) in the limit of a large, steady wave. We use a hydrodynamic solver to find a numerical relationship between the curvature, velocity, and acceleration of the detonation wave that describes the transition between the limits in the ideal and Mie-Gruneisen equations of state.

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CP23

Turbulent Mix in Numerical Simulations for ICF Capsules

We study the turbulent mixing zone in an Inertial Confinement Fusion (ICF) capsule, with a focus on the Rayleigh-Taylor (RT) unstable deceleration phase of hot spot formation. Our main results are twofold: (i) a "post shot" simulation with modifications to input parameters that better resemble experimental observations and (ii) examination of the resulting hot spot and turbulent mixing zone properties.

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CP23

Continuum Boundary Force Method for Multiscale Modeling of Flows Subject to Slip Boundary Conditions

When fluid flow velocity at fluid-solid interfaces is non-zero, the flow is said to have "slip' at the fluid-solid boundary. This phenomenon is commonly described by the Navier boundary condition or, more generally, Robin-type boundary conditions. Here we propose the Continuous Boundary Force (CBF) method for imposing Robin boundary conditions in Smoothed Dissipative Particle Dynamics (SDPD) simulations. We demonstrated the efficiency and accuracy of the SDPD-CBF method for modeling slip flows subject to the Robin boundary conditions with arbitrary (constant, space-dependent, or non-linear) slip lengths at flat and curved boundaries. Furthermore, the consistent thermal scaling in the SDPD-CBF method allows it to also be used for multiscale modeling, i.e., bridging scales in concurrent coupling from the continuum hydrodynamic scale all the way to the molecular scale.

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CP23

Hydrodynamic Calculations Using Reale: An Arbitrary-Lagrangian-Eulerian Framework with Mesh Reconnection

We examine a new ALE hydro scheme that allows for on-the-fly mesh reconnection based on the Voronoi diagram [Loubere et al, ReALE: A Reconnection-Based Arbitrary-Lagrangian-Eulerian Method, JCP, 2010]. Reconnection allows the mesh to follow Lagrangian features in the flow more closely than standard ALE schemes while avoiding the problem of mesh tangling typical of pure Lagrangian schemes. We outline our methodology for ReALE and present results demonstrating its effectiveness on several challenging compressible hydrodynamic tests.

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CP23

A Smoothed Particle Hydrodynamics Model for Electrokinetic Flows

Theoretic description of electrokinetic phenomena includes the Poisson-Boltzmann equation relating the electric field to ion concentration and Navier-Stokes equations relating the flow velocity to the pressure and electrostatic forces acting on the system. A Lagrangian particle model based on smoothed particle hydrodynamics is proposed to numerically solve the coupled equations. And a fast multilevel pre-conditioned method by means of auxiliary space is incorporated as the linear solver for the associated Poisson equation. The efficiency and accuracy of the proposed model are examined through modeling the electroosmotic flow in microchannels and flow through charged membranes. A good agreement is found in comparison with the corresponding analytical or finite-element solutions. The diffusion-advection equation relating the species mass concentration to flow velocity is then coupled to investigate the influence of surface heterogeneity on electrokinetically driven microfluidic mixing.

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CP24

Mutational History Dominates Clonal Selection Within Evolving Tumors

Natural selection acting on clonal diversity within tumors is thought to drive tumor progression, but details remain obscure. Evolutionary mathematical models of the angiogenic switch predict the emergence of hypovascular necrosis caused by hypertumors—"cheating" clones that freeride on vasculature organized by cooperative clones. Here we show that hypertumors should rarely evolve because the deterministic evolutionary trajectory is overwhelmed by stochastic mutational history. These results highlight mutation pressure as a significant evolutionary force in cancer.

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CP24

Modeling the Progression and Development to Hepatocellular Carcinoma for Hepatitis C Virus Infection

The mathematical model considered here is the first attempt to encapsulate the long-term dynamics of hepatitis C virus (HCV) infection and the influence of viral and immune processes in the gradual progression and development to hepatocellular carcinoma (HCC). The key basis for the model formulation is that the long-term implications are random and are very likely caused by cell-mediated immune response. The chances of development of cancer are modeled by way of a stochastic model which takes into account the dynamics over the infection duration. Sampling based simulations show that the development rate of HCC over a period of 40 years is about 9%, which is in consonance with estimates available in literature. Simulations also show that the chance of developing HCC increases linearly along with the length of period of infection at a rate of 2.4 incidents per year for every thousand infected individuals.

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CP24

Quantifying the Relationships among Natural Selection, Mutation, and Stochastic Drift in Multidimensional Finite Populations

The interrelationships of the fundamental biological processes natural selection, mutation, and stochastic drift are quantified by the entropy rate of Moran processes with mutation, measuring the long-run variation of a Markov process. The entropy rate is shown to behave intuitively with respect to evolutionary parameters such as monotonicity with respect to mutation probability (for the neutral landscape), relative fitness, and strength of selection. Strict upper bounds, depending only on the number of replicating types, for the entropy rate are given and the neutral fitness landscape attains the maximum in the large population limit.

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CP24

Competition Between Oysters and Invasive Mussels in the Presence of Water Releases

The Asian green mussel competes with oyster populations in parts of Florida, displacing some reefs in Tampa Bay. However, oysters are more tolerant of salinity changes that can occur, such as when large freshwater releases are made. Releases along waterways can take different forms, with some recent ones being large in volume relative to time. We present an ODE system modeling the population dynamics,

including the effect of fresh water releases. Some numerical results are included.

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CP24

A Mixed-Strategy Game Theoretical Approach for Infectious Disease Prevention by Social Distancing

We describe a population game in which individuals are allowed to decide between adopting different social distancing strategies in order to lower infection risk and maximize payoffs. When the reduction in infection risk is a convex function of the cost of social-distancing, there is a unique pure-strategy game equilibrium. When the reduction in infection risk is not convex, the existence of equilibria becomes more complicated. We will discuss three cases vis--vis different costs of infection.

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CP24

Traveling Wave Fronts in Population and Disease Models with Nonlocal Reaction and Delay

We will discuss the stability of traveling wavefronts for nonlinear reaction diffusion equations with nonlocal reaction and delay. We will prove stability of both non-critical and critical wavefronts, and their rates of convergence. Applications will be made to a host-vector disease model, a generalized Nicholson blowflies model, and a modified vector disease model. This work generalizes results of Lv-Wang and Mei-et-al, and allows us to treat more realistic models.

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CP25

A Q_2−iso−Q_1/Q_1 Immersed Finite Element for Stokes Interface Problems

We present the bilinear immersed finite element (IFE) methods for solving Stokes interface problems with structured Cartesian meshes that is independent of the location and geometry of the interface. Basic features of the bilinear IFE functions, including the unisolvent property, will be discussed. Numerical examples are provided to demonstrate that the bilinear IFE spaces have the optimal approximation capability, and that numerical solutions produced by a Q_2−iso−Q_1/Q_1 method with these IFE functions for Stokes interface problem also converge optimally in both L^2 and H^1 norms.

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CP25

Flow Control by Adjoints and Sensitivities

I will present an algorithm for flow control which is based on the derivation of adjoint equation using Lagrange multipliers. This algorithm involves computing gradient of an user-defined objective function that has the system control settings resulting in sensitivity expressions. Characteristic analysis is incorporated in this methodology to derive sensitivity expressions that yield more information on flow control as compared to sensitivity expressions that are derived without characteristic analysis. Finally, I will show results obtained by applying these algorithms to partial differential equations that model atmospheric flows.

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CP25

A Realizability Preserving Discontinuous Galerkin Method for the M_1 Model for Radiative Transfter in 2D

We consider the M_1 moment model for radiative transfer. In order to ensure well-possedness the moment variables of the model have to satisfy certain realizability conditions. We present the necessary modifications to the Runge-Kutta discontinuous Galerkin method in 2D that ensure realizability of the moment variables. Our goal is to resolve the time evolution of isolated sources or beams of particles in heterogeneous media on unstructured triangular meshes.

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CP25

Optimal Error Estimates of a Linearized Backward Euler Galerkin Fem for the Landau-Lifshitz Equation

We present a fully discrete linearized backward Euler Galerkin FEM for the Landau–Lifshitz equation in which a new linearization is proposed for the gyromagnetic term.

Optimal error estimates are proved almost unconditionally (*i.e.* when the stepsizes h and τ are smaller than given constants). Numerical results are provided to confirm our theoretical analysis and show the unconditional stability of the scheme.

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CP25

A Particle-In-Cell Method Based on An Implicit Wave Solver

A recently developed implicit wave solver removes the CFL condition while maintaining computational cost comparable to explicit wave solvers. We present the application of this wave solver in a particle-in-cell (PIC) method for the simulation of plasmas in an approach that can handle both electrostatic and fully electromagnetic cases. We show the results of some standard one- and two-dimensional electrostatic test problems, and discuss the extension to the fully electromagnetic case.

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CP26

Generalization of Pade Approximation from Rational Functions to Arbitrary Analytic Functions - Applications

We extended the basic idea of Pade approximation to any arbitrary function holormorphic in a neighborhood of the Taylor series expansion point. This provides the flexibility of using other functions in a Pade-type approximation, yielding highly accurate approximations with additional desirable properties such as asymptotic behavior. In this talk, we present applications of our method to approximation of sine/cosine, Fresnel integral functions, representation of band-limited functions, and constructing multiresolution representations, i.e., chirplet decomposition.

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CP26

Analysis of a Singular Integral Equation Modeling Waves Propagating in a Fusion Plasma

A singular integral equation models resonant waves in a fusion plasma. This resonance called hybrid is linked to heating of a magnetic plasma. This presentation is dedicated to the analysis of this equation, see [B. Després, L.-M. Imbert-Gérard, R. Weder, *Hybrid resonance of Maxwell's equations in slab geometry*, J. Math. Pures et Appl., DOI: 10.1016/j.matpur.2013.10.001]. A singular solution is obtained thanks to a limit absorption principle, which provides a formula for the plasma heating.

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CP26

Juxtaposition of Evaporation, Gravity and Darcian Resistance in Seepage Through a Silt Block Adjacent to a Coarse Sand Compartment: Solutions Based on Theory of Holomorphic Functions and Computer Algebra

2-D wicking of soil water is analytically studied by tension-saturated model. Along 3 sides of a transient flow tube the type of boundary conditions is fixed but the 4-th side consists of no-flow boundary and constant-potential segment. In the complex potential domain, the shrinking rectangle is conformally mapped onto the rectangle in the flow domain. The Schwarz-Christoffel formula and Mobius transformation are used. Cauchys problem for an integro-differential equation with respect to an affix of the conformal mapping is numerically solved. Physical and mathematical conditions of solvability of the equation are established. The seepage flow rate as a function of time is presented and related to the classical hydrological taxonomy of evaporation stages. Applications in agricultural engineering, e.g. desiccation of a coarse-textured under-canopy zone of irrigated trees in arid conditions, is related to the developed mathematical model.

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CP26

Unexpected Fooling Functions

We often rely on automatic quadrature rules to compute definite integrals that cannot be expressed in terms of elementary functions. Unfortunately, we have found that nearly all such algorithms can be fooled because their error estimates are based on the difference of two quadrature rules. Using this insight, we have constructed fooling functions that are not particularly spiky, but for which the automatic quadrature rule is grossly incorrect. This highlights the need for better rules.

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CP26

Generalization of Pade Approximation from Ra-

tional Functions to Arbitrary Analytic Functions - Theory

We present a method for extending the basic idea of Pade approximation by using an arbitrary analytic function instead rational functions to match a prescribed number of terms in the Taylor series. The choice of analytic function can be used to construct highly accurate approximations. In this talk, we discuss the theory and error analysis behind our method. Several examples of its application will be discussed in a separate talk.

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CP27

Rate-Limited Sorption in Production Transport Codes

Computational models of contaminant transport are used regularly for designing subsurface environmental remediation systems. In many soils, the contaminant sorbs to the solid matrix in the porous media. As a result, the rate of removal by traditional pump-and-treat flushing is much slower than predicted with equilibrium models. This phenomenon is called rate-limited sorption (RLS) and it is particularly problematic in cases where the contaminant has been in place for a long period of time. Although RLS is well known in academic literature, production models used for field work have failed to incorporate the effect. As a result, remediation designs and cleanup time projections are often inaccurate. In this project, a well-validated production subsurface transport model is modified with a simple analytical model for layers and lenses that incorporates RLS effects with reasonable computational costs. Preliminary results show good agreement with RLS behavior.

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CP27

Fingering Instability in the Presence of Viscoelasticity

With the motivation of understanding the effect of complex rheological properties of complex fluids often used in chemical enhanced oil recovery, we study linear instability of the displacement of a visco-elastic complex fluid and quantify the effect of elasticity on fingering instability. An exact formula is provided which shows that the elasticity has a destabilizing effect on fingering instability. Relevance of these results to chemical EOR will be discussed.

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CP27

Iterative Algorithms for Geosounding Inversion

For most of Geosounding problems, an iterative scheme is usually implemented after linearization of forward equations. Bachmayr and Burger propossed iterative algorithms for TV functionals. Those iterative algorithms are based on Bregman distance, that can be interpreted as a generalization of the mean-square distance for general functionals. In this contribution, several novel algorithms for nonlinear inversion of electrical, electromagnetic and resistivity soundings based on Bregman iterations are presented. Results are reported of algorithm implementation for several geosounding methods applying Bregman distance to minimize the TV and MS functionals. The linear approximation for electromagnetic soundings at low induction numbers is implemented on the inversion algorithm. A comparison of developed models for Bregman based algorithms with those obtained with a linear programming package is also presented for synthetic and field data.

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CP27

A Higher-Order Robert-Asselin Type Time Filter

We propose and analyze a higher-order Robert-Asselin (hoRA) type time filter for weather and climate models. While requiring the same amount of computational effort as the Robert-Asselin-Williams filter, the hoRA filter effectively suppresses the leapfrog schemes computational modes and achieves third-order accuracy. The hoRA filter is shown to be suitable for long-time simulations. In addition, the filter is non-intrusive, and so it would be easily implementable in the existing legacy codes.

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CP27

Coupled Multi-Physics Analysis of Caprock Integrity and Joint Reactivation During Co_2 Sequestration

Structural trapping beneath a low-permeable caprock layer is the primary trapping mechanism for long-term subsurface sequestration of CO_2. We modeled the effects of caprock jointing on the caprock sealing. The modeling effort uses a 3D-FEM based coupled multiphase flow and ge-

omechanics simulator. Various injection schedules as well as caprock jointing configurations within a proto-typical sequestration site have been investigated. The resulting leakage rates through the caprock and fault are compared to those assuming intact material.

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CP27

Modeling of Arctic Melt Ponds and Sea-Ice Albedo-Feedback

We study possibility of the climate system to pass through a bifurcation point - irreversible critical threshold as the system progresses toward ice-free summers. This study is based on the nonlinear phase transition model for melt ponds and bifurcation analysis of a simple climate model with the positive sea ice - albedo feedback as a key mechanism potentially driving the system to the bifurcation point.

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CP28

Multi-Echelon Supply Chain Inventory Optimization: An Industrial Perspective

Mathematical programming based multi-echelon inventory optimization models developed in the literature quantify uncertain demand or lead time assuming a Normal or Poisson distribution. We demonstrate how such assumptions can severely impact and underestimate optimal inventory, and discuss the drawbacks of mathematical programming approaches. We present a novel simulation-optimization framework that not only generates more accurate results by bootstrapping historical data, but is also versatile to capture non-standard inventory policies and decisions. Industrial examples are presented.

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CP28

Single Machine Scheduling Problem with Interval Processing Times

In this paper, the single machine scheduling problem with uncertain and interval processing times is addressed with the objective of minimizing mean weighted completion time. Some polynomial time heuristics, utilizing the bounds of processing times, are proposed. The proposed and existing heuristics are compared by extensive computational experiments. The computational results indicate that the proposed heuristics perform significantly better than the existing heuristics in terms of both error and computation time.

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CP28

Computing Spectra of Laplace Beltrami Operator Using Cylindrical Radial Basis Functions

The spectrum of the Laplace-Beltrami (LB) Operator is known to provide an intrinsic shape signature for 3D shape matching. Given point clouds on a 2 manifold, we utilize a novel cylindrical Radial Basis function to efficiently approximate the surface and compute the Eigen values of the LB operator. At the end, we perform numerical tests to demonstrate the generality and efficiency of our method

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CP28

Sub-Linear Sparse Fourier Algorithm for High Dimensional Data

In this talk, we discuss how to implement a sub-linear sparse Fourier algorithm on data in high dimensional space. We already have the efficient algorithm with O(klogk) runtime for one dimensional problem with k data. We propose a method to embed higher dimensional data in lower space without overlap so that the existent algorithm is applicable to modified data. In this way, we can retain the computational efficiency. It can be shown theoretically and computationally.

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CP28

Interpolation Using the Min Kernel

We find a relationship between the second derivative of a function $f \in C^2[0,b]$, such that $f(0) = 0$, and the coefficients c_j obtained from the interpolation problem $S_f(x_j) = f(x_j)$ at points $x_j, j = 1,\ldots,n$ where $x_j \in (0,b]$, $S_f(x) = \sum_{j=1}^{n} c_j K(x,x_j)$, and K is the min kernel $K(x,z) = \min(x,z)$. We find an integral representation formula, then, adding the boundary condition $f'(b) = 0$, show that $\min(x,z)$ is the Green's function for the Laplacian, and we give an elementary derivation of the native space of the min kernel.

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CP28

On the Entringer and Slater Problem

In 1981, Entringer and Slater proposed the problem of determining $\Psi(r)$, where $\Psi(r)$ is the maximum number of cycles in a connected graph G of order p with q edges and $r = q - p + 1$ (see Aldred R. E. L., Thomassen Carsten, On the maximum number of cycles in a planar graph, J. Graph Theory 57 (2008), no. 3, 255–264). In this talk, some results on this problem and related conjectures are summarized.

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CP28

Tractability of Function Approximation Problems with General Kernels

This talk addresses the problem of approximating functions belonging to a reproducing kernel Hilbert space $\mathcal{H}$. Often convergence rates deteriorate quickly as the dimension of problem increases. Such a behavior is known as the curse of dimensionality. Therefore it is desirable to have dimension independent convergence rates, which corresponds to the concept of strong polynomial tractability. We study the conditions for strong tractability on more general kernels of product form. The shape parameter, γ_ℓ, governs the horizontal scale of a function in $\mathcal{H}$ with respect to the variable x_ℓ. We also introduce a parameter α_ℓ, which governs the vertical scale of the function with respect to the variable x_ℓ. The exponent of strong tractability depends on how quickly the sequence $(\alpha_\ell\gamma_\ell)_{\ell=1}^{\infty}$ tends to zero.

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CP29

An Adaptive Mesh Strategy for Convection Diffusion Problems

It is well known that whenever central finite difference schemes (second order or higher order central schemes) are applied to solve convection diffusion singularly perturbed problems (SPP) numerically on uniform meshes, non physical oscillations observed in the numerical solution and their magnitude increases in the layers (boundary and interior) regions. The presence of these large non physical oscillations in the approximated solution shows that central finite difference operators on the uniform meshes are unstable. To eliminate these oscillations while retaining the order of accuracy, one needs either a fine mesh at the layer. This maybe done either via uniformly fine meshing or via an adaptive mesh strategy. In this paper, a new adaptive mesh strategy has been developed for solving SPP with higher order central compact schemes. Our strategy uses a novel, entropy-like variable as the adaptation parameter for convection diffusion SPP.

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CP29

Are Spectrally-Accurate Radial Basis Functions Obsolete? Gaussian-Mollified Polynomial Interpolation

Spectrally-accurate radial basis functions (RBFs) such as Gaussians often succeed where polynomial interpolation fails because of the Runge Phenomenon. Why? Comparative analysis of RBF and polynomial cardinal functions (nodal bases) shows that RBF cardinals are much more localized. This motivated us to abandon RBFs in favor of Gaussian-mollified polynomial cardinal functions: much more accurate, cheaper to construct and much better conditioned than RBFs. Using potential theory, we prove an exponential, geometric rate of convergence. On a uniform grid, the Runge Phenomenon is not completely annulled, but the Runge Zone is an order of magnitude smaller than for polynomial interpolation. Applications to solving differential equations, especially in complicated geometry, are in progress. A note was published as "Hermite Function Interpolation ..., *Appl. Math. Letters*, **26**, 10, 995-997 (2013).

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CP29

Solutions of Boltzmann Equation for Simulation of Particle Distributions in Plasmas

We are investigating the time evolution of the electron and excited state distribution functions. We solve the time dependent Boltzmann equation to overcome some typical limitations of modeling high pressure plasmas using Monte Carlo methods. Here we focus on the numerical approach to solving the time dependent Boltzmann equation using a multi-term approximation of the electron distribution function. We also compare Boltzmann results for electron distribution evolution against multiple plasma simulations using experimental collisional cross-section data.

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CP29

Investigation and Numerical Solution of Initial-Boundary Value Problem to One Nonlinear Parabolic Equation

In the presented work the difference scheme for specific initial-boundary value problem to the following nonlinear parabolic equation

$$\frac{\partial U}{\partial t} = a\left(x,\, t\right) \frac{\partial^2 U}{\partial x^2} + U^3 + f\left(x,\, t\right)$$

is investigated. The coefficient $a\left(x,\, t\right)$ is required to be continuous and positive. The function $f\left(x,\, t\right)$ is required to be continuous. For the mentioned difference scheme the theorem of convergence of its solution to the solution of the source problem is proved. The rate of convergence is established and it is equal to $O\left(\tau + h^2\right)$. The corresponding numerical experiments are conducted which confirm the validity of the theorem.

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CP29

Coupled Orbital And Thermal Evolution of Major Uranian Satellites

We have developed a model of the orbital and thermal evolution of the five major Uranian satellites over millions of years. The model consists of detailed ordinary differential equations for the orbital evolution coupled to the one-dimensional heat equation for the thermal evolution. We present preliminary results that show how the different terms in the orbital equations such as the oblateness of Uranus affect the orbital semi-major axis and eccentricity of the satellites.

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CP29

A New Optimal Error Analysis of Characteristics-Mixed Fems for Miscible Displacement in Porous Media

In this talk, we establish unconditionally optimal error estimates for a modified method of characteristics with a mixed finite element approximation for the miscible displacement problem in R^d $(d = 2, 3)$, while all previous work required certain time-step restrictions. By introducing a characteristic time-discrete system, we prove that the numerical solution is bounded in $W^{1,\infty}$-norm unconditionally. Thus, optimal error estimates can be obtained in a traditional way. Numerical results are presented to confirm our theoretical analysis.

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CP30

The Heuristic Static Load-Balancing Algorithm Applied to the Community Earth System Model

We propose to use the heuristic static load-balancing algorithm for solving load-balancing problems in the Community Earth System Model, using fitted benchmark data as an alternative to the current manual approach. The problem of allocating the optimal number of CPU cores to CESM components is formulated as a mixed-integer nonlinear optimization problem which is solved by using an optimization solver implemented in MINLP/MINOTAUR. Our algorithm was tested on 163,840 cores of IBM Blue Gene/P.

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CP30

Roadmapping An Obstacle Forest

A growing spectrum of applications targeted for autonomous vehicles drives demand for robust path planners. Environment obstacle information determines route selection in cluttered domains but is only partially exploited by sample-based algorithms. A geometric terrain-based roadmapping approach is discussed that builds, explores and updates Morse navigation functions for forests of obstacle trees. Exploiting a known mathematical characterization of valleys and ridges on the function landscape, a high-level roadmap connecting landscape critical points is constructed.

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CP30

Optimal Control Approach and Numerical Methods for Constrained Smoothing Splines

Constrained smoothing splines are an efficient array of estimators, whose performance often surpasses that of their unconstrained counterparts. The computation of smoothing splines subject to general dynamics and control constraints and initial state constraints is considered. The optimal control formulation of such splines is developed. Several algorithms to compute these splines, including a directional derivative based nonsmooth Newton method, are introduced. The convergence analysis of these algorithms and numerical examples are presented.

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CP30

A Cut Approach for Solving the Single-Row Machine Layout Problem

A cut approach is developed for the machine configuration in a single-row linear layout, with objective to minimize the total material movement cost. We show that the above equidistant linear layout problem is equivalent to the locale network problem by graph theory. The minimum cut, which has the minimum capacity in each locale network, is the corresponding optimal layout that minimizes the material handling cost. The computational complexity of the cut approach is O(n3), where n is the number of workstations in the layout problem. In addition, the non-equidistant linear layout problem can be transformed into an equidistant linear layout problem.

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CP30

Study of Weak Stationarity for a Class of Stochastic Mpcc Problems

In this talk we shall discuss the weak stationarity for a particular class of stochastic mathematical programming problem with complementarity constraints (SMPCC, for short). Our aim here is to show why concept of weak stationarity is important for SMPCC problems even if the problem data is smooth. In fact, a well known technique to solve stochastic programming problems, namely sample average approximation (SAA) method will show the strength of weak stationarity for SMPCC problems.

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CP30

Real-Time Power Dispatch with Renewables Using Stochastic Admm

Leveraging stochastic programming techniques, energy management problems are formulated to account for the intrinsically stochastic availability of renewable energy sources. Both economic dispatch and demand response setups are considered to minimize the microgrid net cost. Based on the stochastic alternating direction method of multipliers (ADMM), a novel decentralized solver with guaranteed convergence is developed for real-time power dispatch. Numerical tests illustrate the merits of the novel approach.

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CP31

On the Existence of Classical Solutions for a Two-Point Boundary Value Problem for the Navier-Stokes Equations

We consider the motion of a liquid surface between two parallel surfaces that are non-ideal, and hence, subject to contact angle hysteresis effect. This effect implies that the contact angle of the capillary surface at the interface is set-valued. We study the problem of existence of classical solutions to the two point boundary value problem in time whereby a liquid surface with one contact angle is deformed to another with a different contact angle.

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CP31

High-Order L-Stable Schemes for the Nonlinear Parabolic Equation Using Successive Convolution

We present a numerical implementation of an L-stable, 3rd order accurate solution of the Cahn-Hilliard model using successive convolution combined with the high order multi-derivative time integrators. The primary advantage is that the operators can be computed quickly and effectively with various boundary conditions using parallel computing.

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CP31

A Scalable, Parallel Implementation of Weighted, Non-Linear Compact Schemes

Weighted, non-linear compact finite-difference schemes, such as the CRWENO scheme (Ghosh and Baeder, SIAM J. Sci. Comput., 2012) and the hybrid compact-WENO scheme (Pirozzoli, J. Comput. Phys., 2002), are well suited for the numerical solution of compressible, turbulent flows. We propose a scalable, parallel implementation of these schemes based on an iterative sub-structuring of the tridiagonal system. We apply our algorithm to benchmark flow problems and demonstrate its scalability on extreme-scale computing platforms.

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CP31

Robust Design of Boundary Conditions for Stochastic Incompletely Parabolic Systems of Equations

We consider an incompletely parabolic system in one space dimension with uncertainty in the boundary and initial data. Our aim is to show that different boundary conditions gives different convergence rates of the variance of the solution. This means that we can with the same knowledge of data get a more or less accurate description of the uncertainty in the solution. A variety of boundary conditions are compared and both analytical and numerical estimates of the variance of the solution is presented.

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CP31

Multilevel Monte Carlo Finite Element Method for Time-Dependent Wave Equation

We propose multilevel Monte Carlo Finite Element method (MLMC-FEM) for time-dependent stochastic wave equation. Our method leads to decrease to log-linear work and memory in the number of unknowns of a single level calculation of the deterministic wave equation. We analyze the MLMC-FEM of the solution based on the nested mesh for Finite Element spaces.

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CP31

Pointwise Estimate for Elliptic Equations in Periodic Perforated Domains

Pointwise estimate for the solutions of elliptic equations in periodic perforated domains is concerned. Let ϵ denote the size ratio of the period of a periodic perforated domain to the whole domain. It is known that even if the given functions of the elliptic equations are bounded uniformly in ϵ, the $C^{1,\alpha}$ norm and the $W^{2,p}$ norm of the elliptic solutions may not be bounded uniformly in ϵ. It is also known that when ϵ closes to 0, the elliptic solutions in the periodic perforated domains approach a solution of some homogenized elliptic equation. In this work, the Hölder uniform bound in ϵ and the Lipschitz uniform bound in ϵ for the elliptic solutions in perforated domains are proved. The L^∞ and the Lipschitz convergence estimates for the difference between the elliptic solutions in the perforated domains and the solution of the homogenized elliptic equation are derived.

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MS1

Network Adaption for Leader-Follower Networks

We examine a networked multi-agent system running consensus susceptible to mis-information from its environment. The influenced dynamics are modeled with leader-follower dynamics and the impact of the foreign input is measured through the open loop $\mathcal{H}_2$ norm of the network dynamics. The measure has a graph-based effective resistance interpretation which allows one to reason about the graph's topological robustness. Consequently, to dampen the external disturbances, decentralized game-theoretic and online edge rewiring methods are proposed.

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MS1

On Leader Selection for Performance and Controllability

A standard approach to controlling multi-agent systems is to select a subset of agents, denoted as leaders, that are directly controlled in order to steer the remaining (follower) agents to a desired state. Approaches to selecting the leader agents currently depend on the design criteria of the system, with continuous optimization techniques employed to guarantee performance and robustness to disturbances, and discrete optimization used to ensure controllability, and hence do not give optimality guarantees for joint selection based on performance and controllability. I will present a unifying approach to leader selection in multi-agent systems based on both performance (e.g., robustness to noise and convergence rate) and controllability. My key insight is that leader selection for joint performance and controllability can be formulated within a matroid optimization framework, implying provable guarantees on the optimality of the chosen leader set. Furthermore, I define a novel graph controllability index, equal to the cardinality of the largest controllable subgraph from a given leader set, and prove that it is a submodular function of the leader set, leading to a submodular relaxation of the problem of achieving controllability.

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MS1

Joint Centrality and Optimal Leader Selection in

Noisy Networks

We discuss the leader selection problem in a model where networked agents, subject to stochastic disturbances, track an external signal. The optimal leader set minimizes steady-state variance about the external signal. We prove the single optimal leader is the agent with maximal information centrality and show the optimal set of m leaders maximizes a measure of joint centrality. Finally, we solve explicitly for optimal leader locations in special cases.

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MS1

Leader Selection in Noisy Multi-agent Systems: A Resistance Distance Approach

We select a number of agents and control them to effectively reject noise in multi-agent systems. This optimization problem is equivalent to grounding nodes in resistance networks such that total effective resistance is minimized. For structured networks in which resistance distances have analytical expressions, we obtain globally optimal selection of leaders. For unstructured networks in which resistance distances can be computed efficiently, we speed up existing greedy algorithms by exploiting sparsity techniques. We illustrate our results with several examples.

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MS2

Bayesian Estimation for Mixtures of Linear Subspaces with Variable Dimension

We assume i.i.d. data sampled from a finite mixture distribution over variable dimension linear subspaces. An embedding of linear subspaces onto a Euclidean sphere allows us to define a joint prior on each subspace and its dimension. The embedding and use of a Gibbs posterior yield model parameter estimates.

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MS2

Distributed Coordinate Descent Method for Learning with Big Data

In this paper we develop and analyze Hydra: HYbriD coordinAte descent method for solving loss minimization problems with big data. We initially partition the coordinates (features) and assign each partition to a different node of a cluster. At every iteration, each node picks a random subset of the coordinates from those it owns, independently from the other computers, and in parallel computes and applies updates to the selected coordinates based on a simple closed-form formula. We give bounds on the number of iterations sufficient to approximately solve the problem with high probability, and show how it depends on the data and on the partitioning. We perform numerical experiments with a LASSO instance described by a 3TB matrix.

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MS2

Efficient Quasi-Newton Proximal Method for Large Scale Sparse Optimization

Recently several methods were proposed for sparse optimization which make careful use of second-order information [10, 28, 16, 3] to improve local convergence rates. These methods construct a composite quadratic approximation using Hessian information, optimize this approximation using a first-order method, such as coordinate descent and employ a line search to ensure sufficient descent. Here we propose a general framework, which includes slightly modified versions of existing algorithms and also a new algorithm, and provide a global convergence rate analysis in the spirit of proximal gradient methods, which includes analysis of method based on coordinate descent.

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MS2

Nomad: Non-Locking, Stochastic Multi-Machine Algorithm for Asynchronous and Decentralized Matrix Factorization

Abstract not available at time of publication.

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MS3

Krylov Subspaces for Approximation of the Spectral Embedding

Spectral embedding problems are solved with truncated spectral decompositions (tSDs); approximation of the tSD may allow for substantial compute savings. Minimal Krylov subspaces have been advocated as tSD alternatives; minimal Krylov subspaces present the greatest potential for compute savings over the tSD, but they also have nontrivial approximation error. We observe that this error is due both to lack of convergence of eigenvalues used in the spectral embedding and convergence of undesired eigenvalues from the opposite end of the spectrum. We also note that eigenvalue approximations may be far more converged than canonical error bounds suggest. We propose preconditioning to produce lower-error minimal Krylov subspaces without incurring much extra computational cost. We demonstrate polynomial preconditioning for approximations of the spectral embedding and develop error bounds for more tightness. These results hint towards minimal Krylov subspace-specific preconditioners.

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MS3

Algebraic Distance on Graphs with Applications to Large-Scale Optimization and Data Analysis

Measuring the connection strength between vertices in a graph is one of the most important concerns in many numerical tasks in graph mining. We consider an iterative process that smooths an associated value for nearby vertices, and we present a measure of the local connection strength (called the algebraic distance) based on this process. Algebraic distance is attractive in that the process is simple, linear, and easily parallelized.

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MS3

Numerical Analysis of Spectral Clustering Algorithms (SCAs)

An SCA employs eigensolves to cluster vertices and edges so that graph topology is better understood. Given a graph, a desired cluster type, and an SCA, how many eigensolver iterations are required for the constituent eigenproblems to have adequate data mining quality? We present in-depth analysis of the simplest cases: power method applied to synthetic data mining problems, with an eye for developing convergence theory for real-world problems and faster iterative methods.

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MS4

Pressure Forcing and Time Splitting for Discontinuous Galerkin Approximations to Layered Ocean Models

This work concerns the application of DG methods to the numerical modeling of the general circulation of the ocean. One step performed here is to develop an integral weak formulation of the pressure forcing that is suitable for usage with a DG method and with a generalized vertical coordinate that includes level, terrain-fitted, and isopycnic coordinates as examples. The computation of pressure at cell edges is facilitated by some ideas that are also used for barotropic-baroclinic time splitting. This formulation is tested, in special cases, with some computational experiments and with analyses of well-balancing, dispersion relations, and numerical stability.

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MS4

Analysis of Adaptive Mesh Refinement for Imex Discontinuous Galerkin Solutions of the Compressible Euler Equations with Application to Atmospheric Simulations

We investigate the performance of a tree-based AMR algorithm for the high order discontinuous Galerkin method on quadrilateral grids with non-conforming elements. We pay particular attention to the implicit-explicit (IMEX) time integration methods and show that the ARK2 method is more robust with respect to dynamically adapting meshes than BDF2. Preliminary analysis of preconditioning reveals that it can be an important factor in the AMR overhead.

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MS4

A Unified Discontinuous Galerkin Approach for Solving the Two- and Three-Dimensional Shallow Water Equations

In this talk, we present a novel discontinuous Galerkin (DG) method that provides a unified approach for solving the two- (depth-integrated) and three-dimensional shallow water equations. A key feature of the developed DG method is the discretization of all the primary variables using discontinuous polynomial spaces of arbitrary order, including the free surface elevation. In a standard Cartesian-coordinate system, this results in elements in the surface layer having mismatched lateral faces (a staircase boundary). This difficulty is avoided in the current method by employing a sigma-coordinate system in the vertical, which transforms both the free surface and bottom boundaries into coordinate surfaces. The top sigma coordinate surface, which corresponds to the free surface, is discretized using triangular and/or quadrilateral elements that are extended in the vertical direction to produce a three-dimensional mesh of one or more sigma layers of triangular prism and hexahedral elements. The polynomial spaces over these elements are constructed using products of Jacobi polynomials of varying degrees in both the horizontal and vertical directions. The DG approach is unified in the sense that in the case of a single sigma layer and a piecewise constant approximation in the *vertical*, the method collapses to a "standard" DG method for the two-dimensional, depth-integrated shallow water equations. The approach also makes use of new (in many cases optimal) sets of nonproduct integration rules and strong-stability-preserving time steppers that have been specifically designed for efficient calculation when used with DG spatial discretizations. The efficiency, robustness and h (mesh) and p (polynomial order) convergence properties of the method will be demonstrated on a set of test cases.

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MS4

A Discontinuous Galerkin Non-Hydrostatic Model with An Operator-Split Semi-Implicit Time Stepping Scheme

A new two-dimensional non-hydrostatic (NH) DG model (compressible Euler or Navier-Stokes system) based on efficient spatial discretization has been developed on (x, z) plane. However, the fast-moving acoustic waves together with a high aspect ratio ($\Delta x = 1000\Delta z$) between the horizontal and vertical spacial discretization impose a stringent restriction on explicit time-step size for the resulting ODE system. We consider a semi-implicit time-split method which employs so-called *horizontally explicit and vertically implicit* (HEVI) approach through an operator-split procedure for the DG discretization. The vertical component of the dynamics, which deals with the acoustic waves and very small grid-spacing (Δz), is solved implicitly while the horizontal part solved in an explicit manner. For the DG model with HEVI time integration, the CFL limit is only restricted to the horizontal grid-spacing (Δx). The model is tested for various NH benchmark test-cases, and the results will be presented in the seminar.

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MS5

My Intertwined Paths: Career and Family

A rich mixture of both career and family characterizes my life during the past twenty years since I earned a PhD in applied mathematics. I'll discuss my intertwined paths – as a researcher at Argonne National Laboratory and as a parent. I will highlight career paths at national laboratories, with emphasis on the diverse opportunities for impact in interdisciplinary computational science. Also, I will reflect on my ongoing choices for work-life balance, including addressing the 'two-body' problem, parenting, and care for aging parents.

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MS5

Beating the Imposter Syndrome

Many competitive and successful students and professionals at times feel like impostors. "I am not as smart as they think I am", or "One sure day, I will disappoint my advisor" are frequently occurring thoughts. In a study of several hundred graduate students at Stanford, we asked about this Impostor Syndrome. I'd like to share some of the results, as well as my own thoughts on how the often negative and sometimes paralyzing thoughts that surface can be turned around. We all need mentors and to connect with a community in our work, and we need this at every career stage. I will tell some stories of successes and failures with these from my own career. I will draw some key conclusions about what to look for in a mentor. And I will reflect on the related topic of community, where the supports and the engagement are bi-directional and dynamic.

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MS5

From Law of Large Numbers...

I would like to share some aspects from my own academic experiences, such as holding positive attitudes, planning and making preparation, and the importance of having good mentors.

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MS5

On the Road Again: My Experience as an Early-career Mathematician

As a mathematician in the transition between postdoc and tenure-track, I will reflect on my experiences thus far and highlight some of the resources that have supported my career. I will also discuss my experience with the academic job market, the two-body problem, pursuing funding opportunities, and seeking a balance between work and personal/family commitments.

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MS5

On the Importance of Good Mentoring and having an Engaging Community

We all need mentors and to connect with a community in our work, and we need this at every career stage. I will tell some stories of successes and failures with these from my own career. I will draw some key conclusions about what to look for in a mentor. And I will reflect on the related topic of community, where the supports and the engagement is bi-directional and dynamic.

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MS6

Parallel Preconditioning for All-at-Once Solution of Time-Dependent Navier-Stokes Optimization Problems

We explore domain decomposition strategies for accelerating the convergence of all-at-once numerical schemes for the solution of time-dependent Navier-Stokes optimization problems on parallel computers. Special attention is paid to developing preconditioners that are robust with respect to parameters, such as the regularization parameter, the Reynolds number, and the timestep size. We describe a parallel preconditioning strategy for these systems that uses domain decomposition algorithms in the time domain and Schur complement approximations for the resulting local saddle point systems. Finally, we present numerical results and discuss possible applications.

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MS6

A Block Diagonal Preconditioner for All-at-Once Solution of Time-Dependent PDE-Constrained Optimization Problems

All-at-once schemes aim to solve all time-steps of parabolic PDE-constrained optimization problems in one coupled computation, leading to exceedingly large linear systems requiring efficient iterative methods. We present a new block diagonal preconditioner which is both optimal with respect to the mesh parameter and parallelizable over time, thus can provide significant speed-up. We will present numerical results to demonstrate the effectiveness of this preconditioner.

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MS6

Fast Iterative Solvers for Reaction-Diffusion Control Problems from Biological and Chemical Processes

In this talk, we develop fast and robust preconditioned iterative methods for solving matrix systems arising from reaction-diffusion control formulations of biological and chemical processes. To construct these methods, we exploit the saddle point structure of the matrices to derive good approximations of the (1,1)-block and Schur complement. For the problems considered, we motivate our recommended preconditioners, discuss parallel solution strategies, and present numerical results to demonstrate the performance of our methods.

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MS6

All-at-Once Multigrid Methods for Optimal Control Problems

In this talk we will discuss the solution of all-at-once multigrid methods for optimal control problems of tracking type with inequality constraints, which might look as follows:

$$\text{Minimize } J(y,u) = \frac{1}{2}\|y - y_D\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}$$

subject to $-\Delta y = u$ on Ω and $y = 0$ on $\partial\Omega$ and *box constraints* (α, y_D and Ω are given). The box constraints might be state constraints ($\underline{y} \leq y \leq \overline{y}$) or control constraints ($\underline{u} \leq u \leq \overline{u}$). One possibility to solve such problems using multigrid methods is to use a (semi-smooth) Newton solver. Here, a standard multigrid method would be used as an solver for linear sub-problems that occur within this iteration. Recently, it was possible to construct and analyze multigrid solvers that can be directly applied to elliptic problems with box constraints (like obstacle problems). Those methods have shown good convergence behavior in practice. In the present talk we will discuss how the ideas of such methods can be extended to control problems.

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MS7

Algorithms That Satisfy a Stopping Criterion, Probably

Numerical algorithms are typically equipped with a stopping criterion where the calculation is terminated when some error or misfit measure is deemed to be below a given tolerance. However, in practice such a tolerance is rarely known; rather, only some possibly vague idea of the desired quality of the numerical approximation is available. Indeed, fast codes for initial value ODEs and DAEs heavily rely on the underlying philosophy that satisfying a tolerance for the global error is too rigid a task; such codes proceed to control just the local error. Another instance of soft error control is when a large, complicated model for fitting data is reduced, say by a Monte Carlo sampling method. If calculating the misfit norm is in itself very expensive then the option of satisfying the stopping criterion only in a probabilistic sense naturally arises. We will discuss this in the context of inverse problems involving systems of PDEs, when many experiments are employed in order to obtain reconstructions of acceptable quality. Major computational savings can then be realized by using unbiased estimators for the misfit function in the stopping criterion.

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MS7

Time Varying RBFs for Wave-Like Solutions of Pdes

We introduce radial basis functions (RBFs) whose time-varying coefficients determine not only the amplitude and position of each RBF but also their shape. The intended use of these Time Varying-RBFs (TV-RBFs) is in the local-in-time representation of low-dimensional approximations of functions that arise in solving spatiotemporal evolution problems; in particular, for time-varying spatially localized solutions with a temporal translation component such as traveling waves, modulated pulses or soliton-like solutions of evolutionary differential equations. This paper is restricted to the one-dimensional spatial case. We also present an algorithm that places the Time Varying-RBFs (TV-RBFs) over spatiotemporal data that may come from experiments, from finely discretized PDE simulations, or even from multiscale, particle-based simulations. It first approximates the function at a single time instant (a temporal snapshot) as a sum of RBFs using a novel weighted minimization that causes each RBF to primarily approximate one of the localized parts of the function. It then extends that approximation to TV-RBFs over a sequence of snapshots of the function at different times. We conclude by discussing the potential uses of these TV-RBFs.

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MS7

On High Index Differential-Algebraic Equations

In this talk we discuss solvability of high index differential algebraic equations. In this context, exponentially faster time scale of evolution of the algebraic variables is pointed out. A numerical method that elucidates the above result by regularizing the Jacobian of the method and producing smoothed solutions is given. The results are illustrated with numerical examples.

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MS7

Sensitivity Analysis of Stochastic Chemical Kinetics

Monte Carlo methods of parametric sensitivity analysis for stochastic dynamics consist of the Girsanov Transformation (GT), Pathwise Derivative (PD) and Finite Difference (FD) methods. The GT differs significantly from the PD and FD methods which are closely related. While each method has its advantages and drawbacks, it has been observed that PD and FD have lower variance than GT in many examples. We provide a theoretical explanation for this in the chemical kinetics context.

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MS8

Optimizing Snake Locomotion in the Plane

We develop a numerical scheme to determine which planar snake motions are optimal for locomotory efficiency, across frictional parameter space. With large transverse friction, retrograde traveling waves are optimal. Our asymptotic analysis shows that the optimal wave amplitude decays as the -1/4 power of the coefficient of transverse friction. At the other extreme, zero transverse friction, we find a triangular direct wave which is optimal. Between these extremes, a variety of locally optimal motions are found, including ratcheting motions. We also extend the study to motion on inclines.

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MS8

From Animal to Robot and Back: Sidewinding on Granular Media

Sidewinders locomote in granular medium through complicated internal shape changes and body-terrain interactions, hence making it is difficult to predict their trajectories. We propose an approach which predicts motions according to body shapes. This approach is built on geometric techniques to prescribe the internal motions and observations from live sidewinders moving on sandy terrain. We demonstrate these ideas on the CMU snake robot.

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MS8

Lessons from Animal Locomotion: Extending Floquet Theory to Hybrid Limit Cycle Oscillators

Animal locomotion is often modeled as a limit cycle oscillator with hybrid (discontinuous) vector field, where classical results of Floquet theory do not apply. We will discuss several recent theoretical results extending Floquet theory to hybrid limit cycle oscillators, as well as ongoing work on numerical/statistical tools for Data Driven Floquet Analysis of legged locomotion systems.

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MS8

Chaotic Scattering during Legged Locomotion on Granular Media

We study locomotion on heterogeneous granular media using laboratory experiments and a granular resistive force theory (RFT). By combining RFT with a multi-body simulator, we model in detail the dynamics of a small open-loop controlled legged sand-running robot. To gain insight into the long-term trajectories, we use cycle expansion theory to study a simplified (scattering potential) model of the locomotor.

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MS9

An Initial Modeling of Fractal Nets for the Sierpinski Gasket

The Sierpienski tetrahedron is obtained by applying an iterated function system (IFS) method to a regular tetrahedron. We give a sketch and algorithm for a folding method that allows us to construct the n-th iteration of a modified Sierpinski gasket, then fold it to form the Sierpienski tetrahedron. We also provide an initial exploration of construction methods for minimal volume objects that retain their surface area under refinement. This idea has potential applications at nanoscale. Advisor: Gregory Fasshauer

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MS9

A Bioinformatic Approach to Cancer Research

The purpose of the study was to identify potential proto-oncogenes and tumor suppressor genes for further research by culture. The R programming language was used to access metadata from the cBio portal. Methylation, mutation, and phosphorylation data were used to distinguish the most likely candidate genes. As a result of this study, two significant candidates were identified, and the oncogenic nature of a family of genes was characterized. Research is ongoing. Advisors: Mingli Yang and Yeatman, Gibbs Cancer Research Center, Spartanburg, SC

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MS9

Billiard Motion of Microorganisms in Confined Domains

Models of ciliated "squirmer" microorganisms indicate that the body rotates passively away from a wall before, during, and after collision. We explore the billiard-like motion of such a body as it swims inside a confined domain. Solutions for stable periodic trajectories inside of regular polygons are derived, and criteria for the existence of other trajectories in complex domains are investigated. The results may provide insight on entrapment and sorting of microorganisms and other active particles. Advisors: Jean-Luc Thiffeault and Saverio E. Spagnolie, UW-Madison

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MS10

Multiscale Modeling and Numerical Simulation of Calcium Cycling in Cardiac Myocyte

In this talk we present the detailed model of the intracellular calcium dynamics in a cardiac myocyte and their efficient numerical techniques. We adopted a detailed CRU model to describe the source functions in the PDE model and the dynamics of the membrane potential is based on the Mahajan membrane Model. We developed a finite element simulator interface for the 452 CRUs arrangement. The numerical convergence of solutions and parallel results are demonstrated.

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MS10

Modeling the Molecular Basis of Calcium Entrained Arrhythmia

Heart disease is the leading cause of death in the developed world and an increasing problem developing nations most often as result of cardiac arrhythmia. Here we examine the cellular and subcellular basis of calcium dependent arrhythmias. In order to understand how calcium dynamics, plays a role in arrhythmogenesis, we have investigated normal and dysfunctional calcium signaling in heart cells at high temporal and spatial resolution using multiscale stochastic models.

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MS10

Cellular Mechanisms of Calcium-Mediated Triggered Activity in Cardiac Myocytes

The main chambers of the heart are made up of electrically coupled ventricular myocytes, which are excitable cells that only transit from the resting to the excited states (fire an action potential) under a finite current stimulus. However, under abnormal conditions, those cells can spontaneously fire a single action potential, or even a burst of several action potentials, after a normal stimulated action potential. This talk will present results of a computational study that sheds new light on the dynamical origin of those arrhythmogenic "afterdepolarizations" by quantifying the relationship of stochastic intracellular calcium dynamics and whole-cell voltage dynamics.

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MS10

Alternans As An Order-Disorder Transition in Heart Cells

Electrical alternans is a beat-to-beat alternation in the amplitude of the electrocardiogram (ECG) which has been shown to be a precursor to various cardiac arrhythmias. In this talk I will argue that nonlinear signaling between stochastic ion channels can explain the onset of alternans. Furthermore, I will present evidence that the transition to alternans occurs via an order-disorder phase transition which exhibits universal features common to a wide range of physical systems.

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MS11

Computing Eigenvalues and Eigenvectors of Symmetric Tensors: A Survey

Eigenvalues and eigenvectors of symmetric tensors have found applications in automatic control, data analysis, higher order diffusion tensor imaging, image authenticity verification, optimization, and other areas. In the past few years several algorithms have been proposed for computing certain eigenpairs of symmetric tensors. In this talk, we will survey these methods. We will also describe some new ideas such as the use of deflation method that can assist the existing algorithms to find other eigenpairs.

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MS11

Dynamical Systems Analysis of Swamps in ALS

The Alternating Least Squares (ALS) algorithm for approximating a tensor by a low-rank tensor is prone to periods of very slow convergence, known as swamps. Although the existence of swamps is well-known and various fixes have been proposed, the mechanisms that cause swamps are mysterious. I will discuss progress on analyzing and understanding swamps using tools from Dynamical Systems.

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MS11

Canonical Polyadic Decomposition for Symmetric Tensor

We propose a method for finding symmetric outer product decomposition for fully and partially symmetric tensor. These are iterative algorithms which are based on matricizations, least-squares and finding roots of quartic polynomials. The methods work well for third-order partially symmetric tensors and fourth-order fully symmetric tensors. Our numerical examples indicate a faster convergence rate than the standard alternating least-squares method.

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MS11

Towards Better Computation-statistics Trade-off in Tensor Decomposition

New approaches for tensor decomposition with worst case performance guarantee have recently emerged. $\mathcal{O}(rn^{d-1})$ is the number of samples required for recovering an $n \times n \times \times n$ d-way tensor that admits a Tucker decomposition with $r \times r \times \ \times r$ core proved for one of these methods called overlapped trace norm. Although this method is computationally very efficient, the rate is rather disappointing. A newer approach called square norm achieves lower $\mathcal{O}(r^{d/2}n^{d/2})$ samples at the cost of higher computational demand. There is also a more theoretical approach that could achieve optimal $\mathcal{O}(rn^d - 1)$ but seem to be computationally intractable. I will overview these recent developments and discuss how we could achieve a better trade-off between what we can provably achieve in terms of statistical accuracy and how much computation we need to spend.

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MS12

Mixing and Transport by Ciliary Flows: A Numerical Study

Motile cilia often serve the dual function of transporting fluid across the cell surface and sensing of environmental cues. The performance of cilia in fluid transport was studied extensively. However, the way by which cilia serve the simultaneous tasks of transport and sensing is less well understood. We use a 3D computational model to examine the transport and mixing properties of ciliary flows. We find that the metachronal wave improves both the transport and mixing rates, often simultaneously. These results suggest that cilia use chaotic advection and mixing as a mechanism to enhance sensing.

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MS12

The Capture of Symbiotic Bacteria from the Environment by Host Ciliated Epithelia

Most, if not all, animals have epithelial cells whose apical surfaces have cilia, elongate mechanosensory appendages that are evolutionarily conserved in their structure and biochemical composition. Cilia often occur in dense, behaviorally- coordinated assemblages along the mucosal surfaces. In these locations, the cilia work in concert with the secreted mucus to capture and translocate suspended materials, notably environmental bacteria. This presentation will focus on what is known about the biology of cilia-bacteria interactions.

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MS12

A Cilia-Driven Hydrodynamic Sieve for Selective Particle Capture

Juvenile Hawaiian bobtail squids reliably capture and isolate a single species of bacteria from inhaled coastal water containing a huge background of other particles. Here I present experimental data showing how arrangement and coordination of the cilia that capture the bacteria create a 3D flow field that facilitates advection, sieving and selective retention of flow-borne particles, including bacteria. These studies may inspire novel microfluidic tools for detection and capture of specific cells and particles.

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MS12

Cilia Generated Flows: Insights from Cell Cultures and Engineered Arrays

The lung stays sterile due to the cilia-generated flow of mucus that sweeps the airway clean. We are studying each aspect of this process: Using a magnetic microbead assay to measure the force developed by individual cilia, using driven microbead rheology to understand strain thickening behavior at nano sized structures, using cell cultures to study biological fluid flow against gravity, and engineering artificial cilia to study directed flow and enhanced mixing in actuated arrays.

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MS13

Frictional and Heat Transfer Characteristics of Flow in Square Porous Tubes of Diesel Exhaust Particulate Filters

In the 1D modeling of flow in the channels of wall-flow monoliths used in diesel particulate filters for engine exhaust emissions control, it is common to use friction coefficients and Nusselt numbers from idealized 2D/3D channel flows. Previously, this idealization suffered from lack of flow through the porous filter walls. As wall flow increases for the simpler geometries of circular tubes and parallel planes, there is a rich literature describing multiple solutions. We extend the practical portion of these results to the computationally challenging, but realistic, square channel geometry that is necessary for mathematical modeling and settle certain long-standing controversies.

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MS13

Solution Verification in Simulations of Drop Impact of Flexible Containers

Solution Verification is an important part of the credibility of a computational model. This activity is focused on determining the rate of convergence of the computed solution as the computational grid gets refined, with the assumption that it will reach an asymptotic regime of convergence. The talk will show some approaches on verifying the solution of a fluid structure interaction problem where flexible container filled with fluid impacts the ground after being dropped.

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MS13

Estimating Shape and Motion Information from

Radar Data

Due to the relatively short microwave wavelengths involved, radar imaging relies on exquisite knowledge of the relative geometry between the antenna(s) and the scene to be imaged (i.e., the target). Radar image formation of non-cooperative targets, such as ships in a rolling sea, is particularly challenging because the target may undergo significant unknown and unpredictable motion. In this talk we discuss our recent progress in estimating arbitrary target motion from radar measurements.

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MS13

Regularization in the Real World

The inverse problem of determining cardiac electrical patterns from measurements on internal or external electrodes has received increasing attention from medical-device companies in recent years. This talk will describe new ideas for regularization methods, simulation and preclinical experiments to evaluate and optimize them, and some of the clinical factors that make reliable solutions more difficult in vivo.

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MS14

Towards τ Adaptivity for Lithosphere Dynamics: Nonsmooth Processes in Heterogeneous Media

We propose a new form of adaptivity based on FAS multigrid, allowing fine grid work to be avoided in regions with nearly-linear behavior, despite arbitrarily rough coefficients. We present preliminary experiments with nonlinear solvers for localized plastic yielding in lithosphere dynamics.

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MS14

Hybrid Parallelism for Large-scale Adaptive-mesh Simulations

With the advent of supercomputers featuring one million processing units or more, maybe the most important guideline for algorithm development is to maximize the concurrency of computational tasks. This is at odds with common solution algorithms for elliptic or hyperbolic PDEs, which are most effective in the mathematical sense but rely on a multilevel structure of causality. In this talk, we discuss options in parallel algorithm design to reduce causality in favor of concurrency.

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MS14

Plate Boundary-resolving Nonlinear Global Mantle Flow Simulations using Parallel High-order Geometric Multigrid Methods on Adaptive Meshes

The simulation of global mantle flow with associated plate motion at global scale is challenging due to the extreme nonlinearity, the viscosity variations, and the different spatial scales inherent in the problem. We discretize the governing nonlinear incompressible Stokes equations using high-order finite elements on highly adapted meshes, which allow us to resolve plate boundaries down to a few hundred meters. Crucial components in our scalable solver are an efficient, collective communication-free, parallel implementation of geometric multigrid for high-order elements, the use of a Schur complement preconditioner that is robust with respect to extreme viscosity variations, and the use of an inexact Newton solver combined with grid continuation methods. We present results based on real data that are likely the most realist global scale mantle flow simulations conducted to date.

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MS14

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MS15

Geometric Locomotion with Passive Internal Degrees of Freedom: Hovering Flight and Passive Swimming

This talk presents a general modeling approach for locomotion dynamics of mobile multibody systems containing passive internal degrees of freedom concentrated into joints and/or distributed along deformable bodies of the system. The approach embraces the locomotion systems bioinspired by animals that exploit the advantages of soft appendages to improve their locomotion performance. It is illustrated through the passive swimming in von Karman Vortex Street (KVS), and the hovering flight with twistable flapping wings.

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MS15

Mapping Effort: Cartographically-Inspired Methods for Representing the Energetic Cost of Locomotion

In kinematic motion planning, Euclidean configuration distance metrics often fail to encode nonlinear effort or power from changing shape. Cartographic techniques can project the distorted configuration coordinates into representations that more accurately portray such distances. We show that the kinematic cartography problem may be reformulated into one of nonlinear dimensionality reduction (NLDR), and compare the results of applying a well-known NLDR technique against a previous spring relaxation algorithm on a three-link low Reynolds swimmer.

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MS15

Numerical-Geometric Analysis of Sandswimming

Sand-swimming, a form of desert burrowing, offers interesting potential as a locomotion mode for robots operating in loose, granular environments. Unfortunately, the computational cost of modeling the relevant physics raises obstacles to a thorough exploration of the system dynamics. Geometric mechanics offers techniques for reducing the complexity of evaluating gaits, thereby offering the potential for exploring a gait design space; unfortunately, these tools have historically been restricted to systems with linear, analytical dynamics. We have recently developed a framework for combining empirical data from nonlinear models with geometric gait evaluation methods. The resulting tools both reduce the computational costs of describing sand-swimming and reveal fundamental aspects of the motion.

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MS15

Coupling of Locomotion Control and Sensing in Biological Systems

The hawkmoth *Manduca sexta* has a keen ability to navigate dense environments with incredible robustness. Although these animals utilize relatively simple, noisy sensors, they harness massively distributed sensing to estimate their state and the state of the surrounding environment. Observability tools give us insight into what information these sensing systems can encode and how locomotion can be used to enhance sensing capabilities.

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MS16

Fully-Automated Multi-Objective Optimization for Fitting Spatial and Temporal Constraints in a Neuronal Model with Real Morphology

We introduce a fully automated optimization methodology for fitting spatially extended neuronal models with multiple time scales. Using multi-objective optimization and targeted experimental protocols, we model a hippocampal CA1 pyramidal cell, which exhibits a sodium channel with widely-separated time constants of recovery from inactivation. Our implementation uses Python to control the NEURON simulator on a multi-core cluster and features a clickable interface to explore the Pareto-optimal front of solutions.

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MS16

Intrinsically Bursting AII Amacrine Cells Drive Oscillations in the Degenerated Rd1 Retina

In retinal degeneration, spontaneous oscillations are observed in retinal output neurons, interfering with signal processing. Using compartmental modeling, based on slice experiments, we show these oscillations are generated by intrinsic bursting of individual AII amacrine cells, which are instrumental in transmitting photoreceptor signals to the output cells. We explain the bursting mechanism by decoupling the fast and slow subsystems, and investigate the bistability between bursting and tonic firing in the model.

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MS16

Synchrony and Phase-Locking of Mixed-Mode Oscillations in a System of Pulse-Coupled Neurons

Our study is motivated by the experimental observation of fast and slow rhythms in the mammalian olfactory system. We develop a minimal model in which the interaction of three relevant populations of neurons is reduced to an effective pulse-coupling amongst a single population of mixed-mode oscillators, and explore the dynamics of this system as a function of the shape and delay of the pulses. We interpret our findings in the context of the observed rhythms.

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MS16

Network Restructuring Guided by Associative Feedback for Enhanced Stimulus Discrimination

The neuronal network performing the initial information processing of olfactory stimuli in mammals exhibits extensive neuronal turnover and a slow restructuring of its connectivity. This network evolution and the activity on this network are modulated by feedback from a network that has properties of an associative memory. Using simple computational models we investigate how these processes allow these coupled networks to learn to discriminate stimuli depending on their familiarity or their association with non-olfactory cues.

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MS17

Hardcore Efficient Computation of Atmospheric Flows Using High-Order Local Discretization Methods

The High-order Adaptively Refined Dynamical Core (HARDcore) composes several compact numerical methods to easily facilitate intercomparison of atmospheric flow calculations on the sphere and in rectangular domains. This framework includes the implementations of Spectral Elements, Discontinuous Galerkin, Flux Reconstruction, and Hybrid Finite Element methods with the goal of achieving optimal accuracy in the solution of atmospheric problems. Several advantages of this approach are discussed such as: improved pressure gradient calculation, numerical stability by vertical/horizontal splitting, arbitrary order of accuracy, etc. The local numerical discretization allows for high performance parallel computation and efficient inclusion of parameterizations. These techniques are used in conjunction with a non-conformal, locally refined, cubed-sphere grid for global simulations and standard Cartesian grids for simulations at the mesoscale. A complete implementation of the methods described is shown with verification test case simulation results based on standard literature.

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MS17

Using the Multilayer Shallow Water Equations for Storm Surge Modeling

Coastal hazards related to strong storms, in particular storm surge, are one of the most frequently recurring and wide spread hazards to coastal communities. In this talk we will present a modification of the standard shallow water model that adds an additional layer to represent the boundary layer of the ocean so that the storm wind forcing is properly taken into account. A demonstration of the utility of this approach will also be presented as applied to Hurricane Ike.

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MS17

Transport Methods for the Community Atmosphere Model's Spectral Element Dynamical Core

Transport algorithms are highly important in atmospheric modeling for climate where hundreds of tracer species must be efficiently transported and it is critical that they satisfy physical bounds and conservation laws. We describe and compare two new transport algorithms that are being developed for the Community Atmosphere Model's (CAM) Spectral Element (SE) Dynamical Core for use on unstructured meshes. The first is a finite-volume based approach where cell intersections between a Lagrangian departure grid and the Eulerian computational grid are computed with the Mesh Oriented Data Base (MOAB). This method is stable for large time steps and is efficient for large numbers of tracer species because the computationally intensive intersection algorithm needs to be called only once per timestep for multiple tracers. The second method is a nodal semi-Lagrangian scheme that has the advantage of directly using the spectral element degrees-of-freedom. This method is coupled with an optimization algorithm to enforce mass conservation and bounds preservation. We evaluate the new methods using several standard two- and three-dimensional transport problems on the sphere and compare to existing approaches.

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MS18

Interpreting the Impact of Constraints for Mean Variance and Cvar Optimization

In this presentation, we study the effect linear constraints have on risk in the context of both mean variance optimization (MVO) and conditional value at risk (CVaR) optimization. Jagannathan and Ma (2003) establish an equivalency between certain constrained and unconstrained MVO problems via a modification of the covariance matrix. We extend their results to both the general case of arbitrary constraints in MVO problems and to CVaR optimization, where the joint density is modified.

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MS18

Addressing the Potential Non-Robustness of Subadditive Portfolio Risk Measures

The modern approach to managing financial market risk is to define an acceptance set for portfolio net asset value at some fixed time horizon according to some probability measure and to impose limits in the current period on the portfolio composition in order to assure acceptable outcomes. Estimating these limits present practical and theoretical challenges (cf Cont et al. [2010]), particularly where outcomes are highly leptokurtotic. We present a concise description of the problem and how it can be addressed.

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MS18

Using Social Influence to Predict Subscriber Churn

With the saturation of mobile phone markets operators focus their energies on identifying potential churners for retention campaigns. Typical churn prediction algorithms identify churners based on service usage metrics, network performance indicators, and demographic information while social influence to churn is usually not considered. We present a churn prediction algorithm that incorporates the influence churners spread to their social peers and show that social influence improves churn prediction and is among the most important factors.

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MS18

Efficient High-Precision Numerical Computation

This talk provides an overview of the methods used to compute numerical functions using high precision in Mathematica. The main focus will be on computation of elementary functions, but applications to special functions will also be mentioned. An outline of the algorithms used will be given together with a description of recent work on more efficient implementation. A comparison with some state-of-the-art special purpose software will also be presented.

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MS19

Changing Directions

We were often told to choose a research area we love. But there are a lot of different kinds of math I love; in fact, any math is fun! In this talk I will share my reflections on how I came to the research area I work in now and factors you can consider when making that difficult choice yourself.

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MS19

Two Jobs, Two Children, and Two Cars: What can Possibly go Wrong?

Some time in the last millennium but it seems longer ago than that my husband and I set out to start a family and find permanent academic jobs, more or less at the same time. Employer-provided daycare, spousal accommodation, and parental leave were yet to be invented. Nonetheless, we benefited from many factors: The novelty of the situation, our willingness to explore different parts of the country and different types of institutions, and our optimism and our determination to do the best we could for our careers and for our family. This talk will summarize our strategies, and will consider what we could have done better.

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MS19

Perspectives of an Assistant Professor

I will reflect on my career path, which did not follow the trajectory I expected. Instead of continuing in a career focused solely on teaching, I moved from being an assistant professor at a teaching university to one at a research university. Along with my career path, I will share the advice I received along the way that shaped this journey. In addition, I will reflect on my experiences of being an assistant professor at two different types of institutions.

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MS20

A Linear Algebra Perspective on Modeling and Computation with Stochastic PDEs

Computational solutions of PDE models with uncertain inputs often begin by representing the randomness in the system with a set of random variables, which become additional coordinates of the PDE solution. One must discretize both the physical domain (space, time) and the random domain (added coordinates) to approximate the solution numerically. Discretization methods yield a host of interesting linear systems to solve. We will compare the linear systems arising in Galerkin methods, pseudospectral methods, and least-squares methods with the goal of offering some practical guidelines for discretization.

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MS20

Strategies for the Efficient Solution of Parameterized or Stochastic PDEs

Many applications, such as stochastic PDEs and uncertainty quantification, lead to a large collection or sequence of parameterized PDEs. Taking into account that we need to solve a collection or sequence of related PDEs can lead to a substantially shorter total solution time (over all systems). We provide a brief overview of methods that help solve systems of parameterized PDEs faster, such as model reduction for parameterized systems, Krylov subspace recycling, and updating preconditioners, and we discuss links between these approaches, and results from recent projects.

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MS20

Computational Complexity of Stochastic Galerkin and Collocation Methods for PDEs with Random Coefficients

We developed a rigorous cost metric, used to compare the computational complexity of a general class of stochastic Galerkin methods and stochastic collocation methods, when solving stochastic PDEs. Our approach allows us to calculate the cost of preconditioning both the Galerkin and collocation systems, as well as account for the sparsity of the Galerkin projection. Theoretical complexity estimates will also be presented and validated with use of several computational examples.

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MS20

Compressive Sensing Method for Solving Stochastic Differential Equations

We solve stochastic partial differential equations (SPDEs) with random coefficients by expanding the solution with generalized polynomial chaos (gPC). We employ the compressive sensing method to recover the coefficients of the gPC expansion given the knowledge that the solution is "sparse". We also combine this method with a special sampling strategy to further increase the accuracy of the recovery of the gPC coefficients. Our method is especially suitable for exploiting information from limited sources.

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MS21

Stochastic Turing Patterns: Analysis of Compartment-based Approaches

Turing patterns can be observed in reaction-diffusion systems where chemical species have different diffusion constants. In recent years, several studies investigated the effects of noise on Turing patterns and showed that the parameter regimes, for which stochastic Turing patterns are observed, can be larger than the parameter regimes predicted by deterministic models. In this talk, the dependence of stochastic Turing patterns on the com-

partment size is investigated. we propose and study a compartment-based model of Turing patterns where each chemical species is described using a different set of compartments. It is shown that the parameter regions where spatial patterns form are different from the regions obtained by classical deterministic PDE-based models, but they are also different from the results obtained for the stochastic reaction-diffusion models which use a single set of compartments for all chemical species. In particular, it is argued that some previously reported results on the effect of noise on Turing patterns in biological systems need to be reinterpretted.

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MS21

Adaptive Accelerated Spatial Stochastic Simulation of Biochemical Systems

Spatial stochastic simulation is an extremely computationally intensive task. This is due to the large number of molecules, which along with the refinement of the discretized spatial domain, results in a large number of diffusive transfers between voxels (sub-volumes). Previously, we presented a novel formulation of the Finite State Projection (FSP) method, called the Diffusive FSP (DFSP) method, for the efficient and accurate simulation of diffusive processes. Using the FSP method's ability to provide a bound on the error, we are able to take large diffusion timesteps with confidence in our solution. We used this to construct an operator split algorithm for spatial stochastic simulation of reaction-diffusion processes that solves diffusion with DFSP and reactions with SSA. However, one of the biggest challenges faced by scientists utilizing DFSP is correct selection of the appropriate operator splitting timestep. A correctly chosen timestep will produce results at the optimum speed without violating the specified error tolerance. Choosing an appropriate timestep requires estimation of the error due to operator splitting. The error is a function of the spatial discretization of the domain, the diffusion coefficients of the molecules within the system, and the stiffness of the chemical reaction channels. Here, we present an extension to the DFSP algorithm that automatically and adaptively selects the appropriate timestep for performance and error control. We demonstrate the utility of this method with a traditional CPU implementation, and its parallel efficiency with a many-core implementation.

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MS21

Stochastic Simulation of Biochemical Networks: Diffusion and Parameter Sensitivity

At the level of a single biological cell, random fluctuations have a significant effect on the biochemistry of the cell. The intrinsic noise in the system with reactions and diffusion is simulated on an unstructured mesh. The parameters in the models will vary due to external sources. We will discuss how diffusion can be modeled on meshes of poor quality and how to include and analyze extrinsic noise in the simulations of an oscillatory system.

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MS21

SParSE: Efficient Stochastic Parameter Search Algorithm for Events

High-performance computing empowers scientists to run large *in-silico* stochastic models that accurately mimic the behavior of the represented system. As the predictive power of such models improve, the need for an algorithm that efficiently determines system configurations for achieving a specific outcome increases. In this presentation, we present a novel parameter estimation algorithm—Stochastic Parameter Search for Events (SParSE)—that automatically computes parameter configurations for propagating the system to produce an event of interest at user-specified success rate and error tolerance.

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MS23

Machine Learning Models for Terrestrial Space Weather Forecasting

Earths magnetosphere experiences loading and unloading processes in response to the incoming energy from the solar wind, creating geomagnetic storms. Predicting these storms is a key priority of space agencies. Due to the scarcity of available data, this system is difficult to simulate with first-principle techniques, inspiring significant research in data-driven models. We investigate the use of advanced graphical machine learning methods including Elman Recurrent Neural Networks and Hidden Markov Models for predicting solar storms. Advisor: Dhruv Batra, Virginia Tech

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MS23

Optimal Control in Time-Varying Velocity Fields using Alpha Hulls

Vehicles in current fields present a difficult optimization problem in charting optimal navigational paths. Recent progress has been made on the general optimal control problem by using front propagation to track the boundary of a reachable set. This work presents a significant advancement by using alpha hulls to dynamically mesh a set boundary in three dimensional space. This method permits higher order optimization, including mixed time-fuel cost metrics and trajectories in three dimensions. Advisor: Shane Ross, Virginia Tech

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MS23

An Extensible Test Matrix Collection

We describe the design and implementation of a test matrix collection. The matrices are grouped into subclasses and their key properties are documented, such as structure, eigenvalues, inverse and condition number. Users can access to matrices by matrix name, by number and by property. They can also include their own matrices by creating new subclasses, which can be easily shared with others. The package is written in Fortran 95 and includes a Python interface. Advisor: Nicholas Higham, University of Manchester

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MS24

Mathematical Modelling of Excitation Contraction Coupling

We present a spatially resolved Ca2+ release unit model. It reproduces experimental findings like gain and gradedness, spark life time and the dependence of release currents and RyR open probability on lumenal Ca2+. A crucial question for the early phase of release is whether the activation of the RyRs is triggered by one or by multiple open LCCs. We address the problem by modelling. We conclude that the activation of RyRs requires multiple open LCCs.

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MS24

Ca2+ Signaling in the Cardiomyocyte: An Atomistic to Cellular Multi-Scale Perspective

Abstract not available at time of publication.

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MS24

Subcellular Calcium Dynamics in a Whole-cell Model of an Atrial Myocyte

Intracellular calcium waves play a crucial role in coordinating contraction of cardiac myocytes. I will present an innovative mathematical modelling approach that allows detailed characterisation of calcium movement within the 3-dimensional volume of an atrial myocyte. Essential aspects of the model are the geometrically realistic representation of calcium release sites and physiological calcium flux parameters, coupled with a computationally inexpensive framework. By translating non-linear calcium excitability into threshold dynamics, we avoid the computationally demanding time-stepping of the full parabolic partial differential equations that are often used to model calcium transport. Our approach successfully reproduces key features of atrial myocyte calcium signalling observed during excitation-contraction coupling. Beyond this validation of the model, our simulation reveals novel observations about the spread of calcium within an atrial myocyte. Furthermore, I will demonstrate that altering the strength of calcium release, the refractoriness of calcium release channels, the magnitude of initiating stimulus, or the introduction of stochastic calcium channel activity can cause the nucleation of pro-arhythmic travelling calcium waves.

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MS25

Complexity and Approximability of Tensor Nuclear Norm

We show that computing the nuclear norm of a 3-tensor is an NP-hard problem. We discuss its approximability and deduce polynomial-time computable upper and lower bounds.

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MS25

Combinatorial Interpretation of the Mesner-Bhattacharya Algebra with Application to Hypermatrix Spectral Decomposition

In this talk we will present an overview of the hypermatrix generalization of matrix algebra proposed by Mesner and Bhattacharya in 1990. In connection with the Mesner-Bhattacharya algebra we discuss a spectral decomposition theorem for hypermatrices, a generalization of the Cayley-Hamilton theorem to Hypermatrices with application to computing new hypergraph invariants.

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MS25

Randomized Methods for Higher-Order SVD

We adapted the work of Halko, Martinsson and Tropp of the randomized range finder in finding the low multilinear rank of tensors.

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MS25

Tensor Linear Discriminant Analysis for Object Recognition

In this talk we explore a tensor based approach to linear discriminant analysis and object recognition. Similar to matrix LDA we determine a basis for projection by minimizing the within class scatter and maximizing the between class scatter. We measure the accuracy of the method and compare to the traditional LDA approach by varying the number of eigenvectors and eigenmatrices used for classification.

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MS26

Leaf Compliance and Foliar Disease Transmission

Foliar diseases in plants are a major cause of crop loss worldwide. Following a recent study which identified various modes of foliar pathogen ejections from contaminated leaves during rainfalls, we here present a theoretical model that rationalizes the effect of foliage compliance on such mechanisms. The laws of fluid dynamics set tight limits on this epidemiological problem of foliar disease transmission and suggest mitigation strategies to the onset of foliar disease spread.

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MS26

Hydrodynamic Contributions to Amoeboid Cell Motility

Understanding the methods by which cells move is a fundamental problem in modern biology. Cell locomotion is integral to physiological processes such as wound healing, cancer metastasis, embryonic development, and the immune response. Recent evidence has shown that the fluid dynamics of cytoplasm can play a vital role in cellular motility. The slime mold *Physarum polycephalum* provides an excellent model organism for the study of amoeboid motion. In this research, we develop a computational model of crawling Physarum. Our model incorporates the effects of the cytoplasm, cellular cortex, the internal cytoskeleton and adhesions to the substrate. Of particlary interest are stresses generated by cytoplasmic flow and how transmission of stresses to the substrate is coordinated. In our numerical model, the Immersed Boundary Method is used to account for such stresses. We investigate the relationship between contraction waves, flow waves, adhesion, and locomotive forces in an attempt to characterize conditions necessary to generate directed motion. Cytoplasmic flows and traction stresses generated by the model are compared to experimentally measured stresses generated by Physarum.

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MS26

Simulation of Fluid Flow Past Conic Obstacles with Applications to Leaves

We present findings from 2 and 3 dimensional simulations of fluid flow past conic obstacles to compare to experiments of leaves in wind tunnels conducted by the Miller Lab. The goal is to study vortex formation at different cone angles, compare boundary layers to asymptotics and if given time potentially measure the impact of elasticity on the obstacle.

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MS26

Plant Leaves Reconfigure into Cone Shapes to Reduce Drag and Flutter

We examine how leaves roll up into drag reducing shapes in strong flows. The dynamics of the flow around the leaves of the wild ginger and tulip poplar are described and compared to simplified sheets using 3D numerical simulations and physical models. In the actual leaf, a stable recirculation zone is formed within the wake of the reconfigured cone. In physical and numerical models that reconfigure into cones, a similar recirculation zone is observed.

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MS27

Demon Design: Circumnavigating Landauer's Limit

Maxwells Demon is a century old thought experiment which has challenged physicists understanding of thermodynamics. We develop a new classical formalism for constructing generalized Maxwellian Demons. We call this new class of systems information engines. These engines use "intelligent" information processing to extract energy from a thermal bath. Although these processes appear to violate the second law of thermodynamics on first inspection, information processing has an energy cost. This cost was once thought to be described by Landauers limit on erasure. We discuss how to design the microscopic and macroscopic architecture of the information engine in order to circumnavigate Landauers Principle, developing a different set of energetic bounds on information processing.

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MS27

Information Processing and the Second Law of Thermodynamics: An Inclusive, Hamiltonian Approach

We obtain generalizations of the Kelvin-Planck, Clausius, and Carnot statements of the second law of thermodynamics for situations involving information processing. To this end, we consider an information reservoir (representing, e.g., a memory device) alongside the heat and work reservoirs that appear in traditional thermodynamic analyses. We derive our results within an inclusive framework in which all participating elementsthe system or device of interest, together with the heat, work, and information reservoirsare modeled explicitly by a time-independent, classical Hamiltonian. We place particular emphasis on the limits and assumptions under which cyclic motion of the device of interest emerges from its interactions with work, heat, and information reservoirs.

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MS27

Towards A Physics of Information: Bit by Bit

Energy and information are fundamental concepts in science, and yet, most would struggle to cite results relating the two, with Landauer's principle, perhaps, being the most well-known. However, there has been renewed interest in relating these concepts, especially as researchers engage the nanoscale. We review information-theoretic measures of memory and organization as developed in computational mechanics, an approach that emphasizes information storage and processing in physical systems. Existing and future applications will also be discussed.

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MS27

Predictive Inference in Non-equilibrium Steady State

Biological sensory systems could be very efficient lossy predictive feature extractors, and a common goal is to engineer systems which learn to extract predictive features of sensory input. One theoretical framework for lossy predictive feature extraction is that of predictive rate-distortion theory. We discuss how to find predictive information curves of output generated by partially-deterministic finite automata. We discuss how input-dependent dynamical systems can extract predictive features of their input automatically. And finally, we ask whether or not an energetically-efficient machine which merely copied the input would necessarily predict the input.

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MS28

Scalable Nonlinear Solvers for Geophysical Problems

Robustness and efficiency of nonlinear solvers, especially for complex multiphysics problems, is a major concern for large scale problems. We present the new framework for nonlinear preconditioning developed in PETSc, and show its application to problem in crustal dynamics from the PyLith package, and lithospheric dynamics from the pTatin3d package.

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MS28

Performance and Scalability of Multigrid Solvers for Geophysical Flow

this talk, we present the abstract concept of hierarchical hybrid grids to design scalable and fast multigrid solvers for the incompressible Stokes that lead to saddle point formulations. Based on a hierarchy of block-wise uniformly refined grids, a semi-structured mesh is obtained that constitutes the starting point for the design and implementation of a massively parallel Stokes solver. In this presentation, we investigate and analyze experiments for Earth Mantle Convection simulations on peta-scale clusters.

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MS28

Computational Environments for Modeling Multiphase Flow, Geochemistry, and Geomechanics

We discuss multiphase models for modeling coupled flow, geochemistry and geomechanics in a porous medium that includes history matching using EnKf. We will present results for a carbon sequestration storage problem and a chemical flood.

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MS29

A Hyperspherical Method for Discontinuity Detection

The objects studied in uncertainty quantification may inconveniently have discontinuities or be contained in an implicitly defined irregular subvolume. Standard techniques are likely to fail; even an adaptive sparse grid method may require excessive sampling to achieve a tolerance. The hypersphere approach detects and unfolds discontinuity surfaces, greatly reducing the influence of highly curved geometry, and allowing good estimates of shape and probabilistic volume.

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MS29

A Hierarchical Stochastic Collocation Method for Adaptive Acceleration of PDEs with Random Input Data

We will present an approach to adaptively accelerate a sequence of hierarchical interpolants required by a multilevel sparse grid stochastic collocation (aMLSC) method. Taking advantage of the hierarchical structure, we build new iterates and improved pre-conditioners, at each level, by using the interpolant from the previous level. We also provide rigorous complexity analysis of the fully discrete problem and demonstrate the increased computational efficiency, as well as bounds on the total number of iterations used by the underlying deterministic solver.

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MS29

Improving Performance of Sampling-Based Uncertainty Quantification on Advanced Computing Architectures Through Embedded Ensemble Propagation

We explore approaches for improving the performance of sampling-based uncertainty quantification methods on emerging computational architectures. Our work is motivated by the trend of increasing disparity between floating-point throughput and memory access speed. We describe rearrangements of sampling-based uncertainty propagation methods to propagate ensembles of samples simultaneously leading to improved memory access patterns and increased fine-grained parallelism. We then measure the resulting performance improvements on emerging multicore architectures in the context of sparse linear algebra.

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MS29

A Generalized Clustering-based Stochastic Collocation Approach for High-dimensional Approximation of SPDEs

We developed a novel generalized clustering-based stochastic collocation (gSC) approach, constructed from, e.g., a latinized hCV tessellation (hCVT), with locally supported hierarchical radial basis function defined over each hCVT cell. This gSC method permits low-discrepancy adaptive sampling according to the input probably density function (PDF), and whose accuracy decreases as the joint PDF approaches zero; effectively approximating the solution only in the high-probability region. Theoretical and computational comparisons to classical sampling and SC methods will also be examined.

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MS30

Matching Exponential and Resolvent Based Centrality Measures in Complex Networks

Centrality measures are used to numerically define the notion of importance of a node to the entire network. In this talk we consider in particular centrality measures based on the matrix exponential and resolvent functions. It has been observed that the ordinal node ranking the resolvent based measure yields can be particular sensitive to the choice of the parameter involved. We show that the parameter can be chosen so that the resolvent measure gives similar rankings to the exponential measure.

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MS30

Anticipating Behavior During Twitter Spikes

We propose and test a novel mathematical model for the activity of microbloggers during an external, event-driven spike. The model leads to a computable prediction of who will become active during a spike. This information is of interest to commercial organisations, governments and charities, as it identifies key players who can be targeted with information in real time. The main expense is a large-scale, sparse linear system solve that is comparable with the cost of computing Katz centrality. We will illustrate the new algorithm on Twitter data around sporting events and TV shows, where spikes in social media activity are driven by external events such as referees' decisions or dramatic plot developments.

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MS30

A Matrix Analysis of Different Centrality Measures

Node centrality measures including degree, eigenvector, Katz and subgraph centralities are analyzed for both undirected and directed networks. We show how parameter-dependent measures, such as Katz and subgraph centrality, can be "tuned" to interpolate between degree and eigenvector centrality, which appear as limiting cases of the other measures. Our analysis gives some guidance for the choice of parameters in Katz and subgraph centrality, and provides an explanation for the observed correlations between different centrality measures.

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MS30

Low-rank Approximation Methods for Ranking the Nodes of a Complex Network

Various network metrics have been introduced to identify the most important nodes in a graph. Some of them are defined as a function of the adjacency matrix associated to the network. We propose a new method to compute such matrix functions, based on a low rank approximation of the adjacency matrix, which allows us to determine a subset that contains the most important nodes, followed by the application of Gauss quadrature to refine the result.

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MS31

A Family of Numerical Methods for Large Scale DFN Flow Simulations avoiding Complex Mesh Generation

A novel optimization method for Discrete Fracture Network (DFN) simulations of subsurface flows is presented. Large scale DFN problems are iteratively split in quasi-independent smaller problems on the fractures that can be efficiently solved on parallel computers, applying several discretization approaches on fractures, with independent meshes. The approach leads to a flexible, efficient and reliable method. The approach is also used for Uncertainty Quantification of flow properties in DFNs.

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MS31

Adaptive Mesh Refinement for Flow in Fractured Porous Media

Discrete fracture models are typically large due to the explicit representation of fractures. For these systems, the fracture connectivity often has the largest impact on flow. In some cases fracture connectivity can restrict the flow to a limited area, leaving large parts of the reservoir essentially inactive. In this work we show how well-driven flow solutions can be used to efficiently adapt the unstructured grid to resolve key flow regions.

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MS31

Meshing Strategies and the Impact of Finite Element Quality on the Velocity Field in Fractured Media

For calculating flow in a fracture network, the mixed hybrid finite element (MHFE) method is a method of choice as it yields a symmetric, positive definite linear system. However, a drawback to this method is its sensitivity to bad aspect ratio elements. For poor-quality triangles, elementary matrices are ill-conditioned, and inconsistent velocity vectors are obtained by inverting these local matrices. Here we present different strategies for better reconstruction of the velocity field.

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MS31

XFEM for Flow in Fractured Porous Media

Simulations of flows in porous media in geological applications are challenging due to geometric complexity and strong variability of properties. To obtain a flexible numerical discretization we employ the XFEM. Grids can be set irrespectively of regions of different permeability since we can represent discontinuous coefficients within elements accurately. Fractures can cut grid elements thanks to suitable enrichments of the pressure and velocity spaces. Finally, $n-1$ dimensional XFEM are employed to treat the intersections between fractures.

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MS32

Mathematical Models of Metabolic Dysfunction in Type 2 Diabetes

Type 2 diabetes is a slowly progressing and complex metabolic disease with a multitude of etiological factors. Although it is primarily caused by reduced cellular uptake of glucose (insulin resistance) and insufficient insulin production (β-cell dysfunction), many of its underlying mechanisms remain unknown. We develop a series of mathematical models to describe cellular and molecular processes involved in the progression of insulin resistance and β-cell dysfunction and discuss implications for metabolic irreversibility and disease onset time.

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MS32

Oscillation of Nabla Dynamic Equations on Time Scales

In this talk we discuss the oscillatory behavior of the second-order nonlinear nabla functional dynamic equation

$$\Big(p(t)y^{\nabla}(t)\Big)^{\nabla} + q(t)f(y(\tau(t))) = 0$$

on a time scale (a nonempty subset of the real numbers) $\mathbb{T}$ with $\sup \mathbb{T} = \infty$. We establish a sufficient and necessary condition which ensures that every solution oscillates. Next we establish the oscillatory equivalence of the above dynamic equation and the second-order nonlinear nabla dynamic equation

$$\Big(p(t)y^{\nabla}(t)\Big)^{\nabla} + q(t)f(y^{\rho}(t)) = 0$$

on time scales. We close with an example.

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MS32

Fetal Heart Rate and EEG Modeling: Predicting Fetal Distress in Labor

During labor, fetal well-being is typically monitored by measuring fetal heart rate (FHR). It is known that more reliable monitoring modalities are needed. To address this, we present a mathematical model which explores the monitoring of two signals, FHR and EEG, as a way to predict fetal distress. Our modeling approach includes blood flow to the heart and brain and incorporates several key features such as, oxygen delivery, blood flow redistribution, blood pressure, chemo and baro-receptor mechanisms.

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MS32

A Biological Application of the Oriented Skein Relation

The tangle model was developed in the 1980's by professors DeWitt Sumner and Claus Ernst. This model uses the mathematics of tangles to model protein-DNA binding. An n-string tangle is a pair (B, t) where B is a 3-dimensional ball and t is a collection of n non-intersecting curves properly embedded in B. In the tangle model for DNA site-specific recombination, one is required to solve simultaneous equations for unknown tangles which are summands of observed DNA knots and links. This presentation will give a review of the tangle model for site specific recombination, discuss another tangle model that utilizes the oriented skein relation for knots and give an application for these models to biological processes.

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MS33

Fast Sweeping Methods for Steady State Problems for Hyperbolic Conservation Laws

Fast sweeping methods are efficient interactive numerical schemes originally designed for solving stationary Hamilton-Jacobi equations. Their efficiency relies on Gauss-Seidel type nonlinear iterations, and a finite number of sweeping directions. We generalize it to hyperbolic conservation laws with source terms. The algorithm is obtained through finite difference discretization, with the numerical fluxes evaluated in WENO fashion, coupled with Gauss-Seidel iterations. High order accuracy and the capability of resolving shocks are achieved. In further study, we incorporate multigrid method to improve the efficiency.

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MS33

Nonlinear Traveling Waves for a Model of the Madden-Julian Oscillation

The Madden-Julian oscillation (MJO) is a planetary-scale wave envelope of cloud and storm activities in the tropics. MJO significantly affects other components of the atmosphere-ocean-earth system. Recently, a nonlinear model is presented for capturing MJO's features. I will present the exact nonlinear traveling wave solutions based on the model's energy conservation. The solution allows for explicit comparisons between features of linear and nonlinear waves, such as dispersion relations and eligible traveling wave speeds.

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MS33

Nonlinear Neutral Inclusions: Assemblages of Spheres and Ellipsoids

If a neutral inclusion is inserted in a matrix containing a uniform applied electric field, it does not disturb the field outside the inclusion. The well known Hashin coated sphere is an example of a neutral coated inclusion. In this talk, we consider the problem of constructing neutral inclusions from nonlinear materials. In particular, we discuss assemblages of coated spheres and ellipsoids.

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MS33

Energy-Conserving Discontinuous Galerkin Methods for the Vlasov-Ampere System

In this talk, we propose energy-conserving numerical schemes for the Vlasov-Ampere (VA) systems. The VA system is a model used to describe the evolution of probability density function of charged particles under self consistent electric filed in plasmas. It conserves many physical quantities, including the total energy which is comprised of the kinetic and electric energy. Unlike the total particle number conservation, the total energy conservation is challenging to achieve. For simulations in longer time ranges, negligence of this fact could cause unphysical results, such as plasma self heating or cooling. In our work, we develop the first Eulerian solvers that can preserve fully discrete total energy conservation. The main components of our solvers include explicit or implicit energy-conserving temporal discretizations, an energy-conserving operator splitting for the VA equation and discontinuous Galerkin finite element methods for the spatial discretizations. We validate our schemes by rigorous derivations and benchmark numerical examples such as Landau damping, two-stream instability and bump-on-tail instability.

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MS34

Bayesian Inference with Reduced-order Models and Statistical Error Estimates

Bayesian inversion for parameterized PDEs requires sampling from the posterior distribution, which can entail thousands of forward simulations; this is infeasible with large-scale models. To make this tractable, we 1) replace the large-scale model with a reduced-order model (ROM), and 2) rigorously account for the ROM error using the novel ROMES method. ROMES provides a statistical model of this error by constructing a stochastic process mapping error indicators (e.g., residual norm) to a distribution over the ROM error.

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MS34

Partial Eigenvalue Assignment in Large-Scale Linear Stochastic Dynamic Systems

The objective of the proposed work is to characterize feedback matrices for large-scale linear dynamic systems within the framework of nonlinear eigenvalue problem and robust design optimization under uncertainty. The proposed formulation takes into account the effects of constraint violations associated with certain risk assessment for the dynamic system under consideration. It is based on the concept of quantiles and tail conditional expectations. Numerical examples will be presented to illustrate the proposed framework.

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MS34

Optimal Sampling of Polynomial Chaos Expansions

We investigate Monte Carlo sampling of random inputs for the estimation of coefficients in a sparse polynomial chaos expansion, with a particular focus on high-dimensional random inputs. Sampling from the distribution of the random variables is typically sub-optimal in a statistical sense. Asymptotic properties of orthogonal polynomials yield sampling schemes with reduced dependence on the order and dimension of polynomial basis. We present alternative sampling schemes including a Markov Chain Monte Carlo sampling with a statistical optimality.

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MS34

High-Dimensional Approximation with Discrete Leja Sequences

We investigate weighted Leja sequences for non-intrusive interpolatory/approximation schemes of differential equations parameterized by a random variable. Leja sequences are attractive for building surrogates of parametric dependence because of their asymptotically optimal properties in the pdf-weighted norm. In this talk we discuss the application and construction of discrete approximations to these sequences, the latter of which involves canonical numerical linear algebra routines and maximum-volume subspace selection.

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MS35

Integration of Molecular Science and Engineering

Electrodeposition is a key process step in the fabrication of high-value products. Deposit formation involves a wide variety of physical phenomena that span multiple time- and length-scales. Although new scientific knowledge at the atomic-scale is revolutionizing understanding, the design of well-engineered products presents significant computational challenges. This presentation describes use of kinetic Monte Carlo and First Passage Time algorithms from an engineering perspective that requires massively iterative optimization calculations based on incomplete fundamental knowledge.

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MS35

Intrinsic and Extrinsic Fluctuations in a Spatiotemporal Oscillatory System

Appropriate modeling and simulation frameworks for studying extrinsic noise in spatial settings will be increasingly important as cell biologists dissect the relative contributions of intrinsic and extrinsic fluctuations to total stochasticity on ever finer scales. Here we present an extension to URDME to incorporate extrinsic noise into a spatial, mesoscopic setting. As an example, the method is demonstrated on a model of experimentally observed, spatiotemporal Min protein oscillations in E. Coli cells. When extrinsic fluctuations are modelled as a coloured noise process the sensitivity of a system may depend critically on the typical lifetime of the noise. This phenomenon is observed here and illustrates the importance of taking the timescale of interacting processes into account when analyzing a models robustness to noise.

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MS35

Multi-Physics Multiscale Simulations for Dusty Proto-Planetary Disks

We develop a numerical package to simulate the interaction between the protoplanetary disks and embedded protoplanets. The disk motion is described as PDEs(hyperbolic, parabolic, and elliptic type). The planet motion is described as ODEs. The coupled system contains multiple length and time scales. Several numerical techniques including multiscale method have been developed to accelerate the time integration. Adaptive mesh refinement and parallel-in-time methods are also used to speed up the calculation.

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MS35

Understanding the Network of Oscillators in the Mammalian Circadian Clock

The mammalian circadian clock is comprised of thousands of heterogeneous intracellular oscillators synchronizing their rhythms via intercellular communication. It is not well understood how such a diverse set of cells synchronizes. Using a mechanistic ordinary differential equation model, we have identified an inverse relationship between intrinsic amplitude and phase response properties as a key factor in synchronization. Using a simple phase-amplitude model, we relate our earlier findings to the ability to synchronize increasingly heterogeneous populations.

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MS36

Inertial Particles in Turbulence, Caustics and Col-

lisions

Abstract not available at time of publication.

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MS36
Capillary Fracture

I will describe the initiation and growth of fractures in gels close to their solid-liquid transition. In experiments, channel fractures form at the surface of the gel, driven by fluid propagating away from a central droplet. Their initiation is governed by two processes. First, surface-tension forces exerted by the droplet deform the gel substrate and break azimuthal symmetry. We model the substrate as an incompressible, linear-elastic solid and characterize the elastic response to provide a prediction for the number of fracture arms as a function of material properties and geometric parameters. Second, a thermally-activated process initiates a starburst-shaped collection of fractures corresponding to this strain-patterning. Once initiated, the fractures grow with a universal power law $L = t^{3/4}$, with the speed limited by the transport of an inviscid fluid into the fracture tip.

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MS36
Low Energy Cardiac Defibrillation

Abstract not available at time of publication.

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MS36
Nonlinear Waves and Wave Turbulence

Abstract not available at time of publication.

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MS37
A Mathematical Model for the Sexual Selection of Extravagant and Costly Mating Displays

The evolution of extravagant and costly ornaments on animals has intrigued biologists since Darwin suggested that female preference for exaggerated courtship displays drives the sexual selection of these ornaments. We propose a minimal mathematical model which incorporates two components of ornament evolution: an intrinsic cost of ornamentation to an individual, and a social benefit of relatively large ornaments within a population. Using bifurcation analysis and perturbation theory, we show that animals will split into two niches, one with large ornaments and one with small, a phenomenon observed in many species.

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MS37
Qualitative and Asymptotic Theory of Detonations

We derive a multidimensional weakly non-linear asymptotic model of detonation waves capable of reproducing the rich nonlinear dynamics observed in solutions of the reactive Euler equations, both in one and multiple space dimensions. Quantitative and qualitative comparison between the asymptotic equations and the full system they approximate are also presented.

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MS37
A Linear Quadratic Programming Method for Nonlinear Model Predictive Control

Nonlinear Model Predictive Control (NMPC) requires iterative approximative solution of optimal control problems. After discretization these are given as nonlinear programs. State-of-the-art solvers use Sequential Quadratic Programming to this end. Several industrial applications demand the solution of Mixed-Integer NMPC Problems with combinatorial constraints leading to Mathematical Programs with Equilibrium Constraints. We investigate an SLEQP method that uses LPs to determine active sets and steps given by a combination of Linear and equality constrained Quadratic Programs.

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MS37
Mathematical Model of Transplant Rejection: Roles of T cells, Antigen Presenting Cells, and Cytokines

A mathematical model of the immune-mediated rejection of transplants predicts a 50% decrease in graft mass within two weeks of transplantation. Effector T cells propagate rejection while regulatory T cells limit it; the model is used to test graft tolerance-promoting interventions. Decreasing the effector T cell translocation rate into the graft typically delays rejection, although this effect depends on relative cytokine concentrations. Doubling the initial number of regulatory T cells delays rejection by two weeks.

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MS37

Solving Differential Algebraic Equations Using Structural Analysis Based Dummy Derivatives

Differential algebraic equations, DAEs, appear frequently in applications involving equation based modelling. A common way of making a DAE amenable to numerical solution is by reducing it to a corresponding (usually implicit) ODE. The signature matrix method instead solves the DAE directly via Taylor series [1]. We draw comparisons between these two different approaches and show the signature matrix method is in some sense equivalent to the dummy derivative index reduction method [2].

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MS37

A Mathematical Model of an Arterial Wall

Elastic arteries are significantly prestretched in axial direction and this has great influence on the mechanical behavior during the pressure cycle. Our study presents results of a simulation of the inflation-extension behavior and comparisson of several different models of the wall. The constitutive parameters and geometries for 17 aortas adopted from the literature were supplemented with initial axial prestretches obtained from the statistics of 365 autopsy measurements.

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MS38

Hamilton-Jacobi Equations for the Continuum Limits of Sorting and Percolation Problems

We show that two related combinatorial problems have continuum limits that correspond to solving Hamilton-Jacobi equations, and give convergent numerical schemes. The first problem is non-dominated sorting, which is fundamental in multi-objective optimization, and the second is directed last passage percolation (DLPP), which is an important stochastic growth model closely related to directed polymers and the totally asymmetric simple exclusion process (TASEP).

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MS38

Fast and Accurate Redistancing Via Directional Optimization

A fast and accurate algorithm for the reinitialization of the signed distance function in two and three spatial dimensions is presented. The algorithm has computational complexity O(N log N) for the reinitialization of N grid points. The order of accuracy of the reinitialization is demonstrated to depend primarily on the interpolation algorithm used. Bicubic interpolation is demonstrated to result in fourth-order accuracy for smooth interfaces. Simple numerical examples demonstrating the convergence and computational complexity of the reinitialization algorithm in two and three dimensions are presented as verification of the algorithm.

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MS38

Numerical Solution of the Second Boundary Value Problem for the Monge-Ampère Equation

The second boundary value problem for the Monge-Ampere equation consists of a fully nonlinear elliptic partial differential equation (PDE) with a global constraint on the image of the gradient map. The state constraint is replaced by a more tractable local PDE on the boundary. Using wide-stencil finite difference schemes, we construct a numerical method that converges to the viscosity solution of the underlying problem.

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MS38

Convergent Filtered Schemes for the Eikonal Equation

The approximation theory of Barles and Souganidis [Asymptotic Anal. 4 (1991), pp. 271-283] guarantees the convergence of numerical schemes to the viscosity solution provided they are monotone, stable and consistent. However, theses schemes are in general only 1^{st} order accurate. Froese and Oberman [Siam J. Numer. Anal. 51 (2013), pp. 423-444] introduced recently convergent filtered schemes which achieve high order where the solutions are sufficiently smooth. In this talk, we construct filtered schemes to the Eikonal equation, present results in one and two dimensions and compare them to the ENO schemes [Siam J. Numer. Anal. 28 (1991), pp. 907-922].

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MS39

Using Krylov Subspace Method for the Canonical Polyadic Decomposition

We propose method based on Krylov subspace methods in finding the minimum sum of rank one tensors. For rank deficient least-squares problems, this iterative method is efficient with respect to the computational cost and memory.

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MS39

Source Apportionment of Time and Size Resolved Ambient Particulate Matter

The proposed weighted alternating least squares method was used to analyze size- and time-resolved particle sample compositional tensor data. The algorithm identified five emission sources: soil, deicing road salt, aircraft landings, transported secondary sulfate, and local sulfate/construction. The largest source associated with the airport operations was aircraft landing that had not been previously considered as a significant source of particles.

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MS39

Stochastic Approximation Algorithms for the Polyadic Decomposition

In a polyadic decomposition, a tensor is written as a sum of rank-1 terms. The computation of this decomposition often involves the minimization of the distance between the tensor and the decomposition. Most iterative algorithms use every known element in each iteration. By using stochastic approximation techniques, only a few points are accessed in each iteration. The number of data point accesses can thus be reduced, which is important in big data applications.

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MS40

Hydrodynamics and Control of Microbial Locomotion

Interactions between swimming cells, surfaces and fluid flow are essential to many microbiological processes, from the formation of biofilms to the fertilization of human egg cells. Yet, relatively little remains known quantitatively about the physical mechanisms that govern the response of bacteria, algae and sperm cells to flow velocity gradients and solid surfaces. A better understanding of cell-surface and cell-flow interactions promises new biological insights and may advance microfluidic techniques for controlling microbial and sperm locomotion, with potential applications in diagnostics and therapeutic protein synthesis. Here, we report new experimental measurements that quantify surface interactions of bacteria, unicellular green algae and mammalian spermatozoa. These experiments show that the subtle interplay of hydrodynamics and surface interactions can stabilize collective bacterial motion, that direct ciliary contact interactions dominate surface scattering of eukaryotic biflagellate algae, and that rheotaxis combined with steric surface interactions provides a robust long-range navigation mechanism for sperm cells.

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MS40

Orientational Order in Two-Dimensional Confined Active Suspensions

Geometric confinement in physical space is important for the studies of the collective motion of suspensions of active swimmers. The reasons are two-fold: motile biological micro-organisms or active colloids are always subject to different types of confinement in the swimming environment; The existence of confinement can have significant effects on the hydrodynamic interactions between the swimmers and thus changes the nature of the collective motion. We focus on the situation when the swimmers are confined between two parallel plates (Hele-Shaw cell) such that the motion of the particles are restricted to two dimensions. In this case, the far-field hydrodynamic effect of a swimmer is no longer given by a force-dipole, which has been used in numerous studies on discrete numerical simulations and continuum theories. Instead, the far-field effect of a confined swimmer is given by a potential-dipole.

Using a potential-dipole model in doubly-periodic domain, we perform numerical simulations to probe into the collective dynamics of confined active suspensions. We show that, depending on whether the swimmers have head-and-tail symmetry, the isotropic suspensions of swimmers can develop either long time polar orientation order, local alignments and non-mobile clusters or combination of the above, which are novel collective behavior compared to swimmer suspensions in unconfined geometries.

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MS40

Surface Interactions in Suspensions of Swimming Cells

Interactions between swimming cells and surfaces are essential to many microbiological processes, from bacterial biofilm formation to human fertilization. However, despite their fundamental importance, relatively little is known about the physical mechanisms that govern the scattering of flagellated or ciliated cells from solid surfaces. In the talk I will reveal recent advances in understanding of flagella interaction with surfaces, provide mechanisms for utilizing our knowledge about these interactions to control swimming of flagellated cells. In addition, I will describe our very recent results on sperm rheotaxis near surfaces. The key focus will be on the experimental results, supported by numerical simulation using minimal models.

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MS40

Modeling of Hydrodynamic Interactions of Large Groups of Swimming Microorganisms in Viscoelastic Fluids

Hydrodynamic interactions of swimming microorganisms can lead to coordinated behaviors of large groups. The impact of viscoelasticity on the collective behavior of active particles driven by hydrodynamic interactions has been quantified with the inclusion of rotational diffusion. Oldroyd-B, Maxwell, and generalized linear viscoelastic modeled are considered as the constitutive equation of the suspending fluid, inspired by some biological fluids. A mean field assumption is used to model the suspension dynamics near an isotropic state. The onset of instability has been quantified by a linear stability analysis in terms of wavenumber, diffusivities, and constitutive equation parameters. Some key results are in contrast to suspensions in Newtonian fluids. The maximal growth rate can occur at a particular wavelength, and diffusion can act to make the system more unstable. Viscoelasticity can also affect the long time dynamics of the continuum equations.

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MS41

Low-Dimensional Dynamics Embedded in Echo-State Networks

Abstract not available at time of publication.

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MS41

Metastability and Coherent Structures in Large Stochastic Neuronal Networks

We will consider stochastic dynamical systems defined on networks where the individual dynamics mimic standard neuronal models, and show that the systems can exhibit various types of coherent and metastable behavior. We will demonstrate that there is a naturally occurring, but non-standard, spectral problem in problems of this type; analysis of this spectral problem will show that its salient features are determined by a certain homology group.

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MS41

Integrate-and-Fire Model of Insect Olfaction

When a locust detects an odor, the stimulus triggers a series of synchronous oscillations of the neurons in the antenna lobe. These oscillations are followed by slow dynamical modulation of the firing rates which continue after the stimulus has been turned off. I model this behavior by using an Integrate-and-Fire neuronal network with excitatory and inhibitory neurons. The inhibitory response of both types of neurons contains a fast and slow component. The fast component, together with the excitation, creates the initial oscillations while the slow component suppresses them and aids in the creation of the slow patters that follow. During the initial oscillations the stimulus can be identified by determining which excitatory neurons participate consistently in every cycle of the oscillations.

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MS41

Generalized Linear Models for Networks of Spiking Neurons

Abstract not available at time of publication.

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MS42

Cytoplasm Rheology and Its Role Cellular Blebbing Dynamics

We present a computational model to describe the dynamics of blebbing, which occurs when the cytoskeleton detaches from the cell membrane, resulting in the pressure-driven flow of cytosol towards the area of detachment and the local expansion of the cell membrane. The model is used to explore the relative roles in bleb dynamics of cytoplasmic rheology, permeability of the cytoskeleton, and elasticity of the membrane and cytoskeleton. We show that the multiphase poroelastic nature of cytoplasm is essential to explain experimental observations.

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MS42

An Analytic Framework for Pairwise Correlations in Active Swimming

In recent years there has been considerable interest in active fluids, such as suspensions of swimming microorganisms. A key observation for such suspensions is the tendency of "pushing" swimmers (typically bacteria, e.g. E. coli) to develop long range orientational correlations; in stark comparison to "pulling" organisms (typically algae, e.g. C. reinhardtii) which tend to remain uncorrelated. This observation is consistent with analytical results in mean field theories for hydrodynamically interacting swimmers, where the uniform isotropic state is stable for pullers but unstable for pushers. However, a mean field theory can not be used to actually predict correlation length scales, as it assumes independence of distinct swimmers. Being able to predict such two-point statistics is an important step in characterizing the macroscopic rheological properties of the suspension as a whole. In this talk an analytical framework for computing the correlations in a simplified phenomenological model for swimming will be discussed.

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MS42

Finite Length Undulatory Swimmers: Whether to Kick Or to Burrow in a Viscoelastic Fluid

We explore finite length undulatory swimmers in viscoelastic fluids. The worm is modeled as an inextensible infinitely thin sheet in 2 dimensions and the swimming is driven using a prescribed target curvature. We look at front-back asymmetries in the prescribed stroke pattern and consider the effect on swimming speed and efficiency. The importance of passive dynamics, where swimmers are given prescribed torques rather than prescribed shapes, is explored. We show that kickers can get a larger boost from viscoelasticity than burrowers.

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MS42

Exploring the Effect of Glass-Forming Sugars on Vesicle Membrane Dynamics During Drying

When immersed in a liquid, certain sugars have a "glass-forming" effect on the liquid at large enough concentration. In particular, the viscosity of the liquid is found to be heavily dependent on the sugar concentration, reaching that of a glass in optimal conditions. These sugars, and their affect on cellular structures, are of interest to the biological community for various reasons, one of which is their use in the preservation of biological material. Whereas cryopreservation stores material using extremely low temperatures to reduce cellular mobility, a new technique named lyopreservation uses the aforementioned glass-forming effect to reduce mobility. However, current attempts to achieve lyopreservation have less than successful. The work discussed in this talk focuses on modeling a single cell undergoing drying similar to that involved in current lyopreservation techniques. This is done by considering a vesicle placed in a fluid containing a spatially varying concentration of sugar. The model incorporates the bending resistance and inextensibility of the membrane, the viscosity dependence on the sugar, the flow of liquid across the vesicle membrane, as well as the surrounding concentration and velocity fields. It is solved using the level set, immersed boundary, and immersed interface methods. The results focus on identifying how the various material parameters affect the vesicle dynamics and attempt to identify ideal regimes for achieving lyopreservation.

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MS43

Qualitative Reasoning with Modelica Models

Qualitative reasoning allows us to reason about physical systems using simplified systems of qualitative differential equations, in a way which preserves important behavioral aspects of those systems. However, a continuing challenge in that work is the construction of appropriate qualitative models of those systems. Meanwhile, designers are increasingly using the Modelica language to create simulation models of proposed designs for numerical simulation. Our group at PARC has addressed the model construction bottleneck of qualitative reasoning by automatically transforming Modelica models into qualitative models. In this talk, we describe that process, and discuss the challenges in abstracting equations into constraints, determining initial conditions and discrete events, and identifying appropriate continuous behavior. We identify places where additional qualitative constraints can be derived from Modelica equations, and describe how we bridge the gaps between Modelica and existing qualitative simulation work on discrete behavior. Our system has been integrated with existing Modelica tools; we describe its potential applications to mechatronic engineering design.

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MS43

Enabling Technologies for Web-Based Engineering Analysis

The web and cloud have become ubiquitous in our everyday lives. The societal impact of these technologies is significant. Everyday, new tools and technologies are introduced to facilitate the creation of web-based applications. But most of these applications are targeted at consumer level applications. Although these applications are driven by very interesting mathematical principles (for machine intelligence, data correlation, etc), they are successful because they use these principles to create a significant impact for non-technical users (i.e. consumers). In the engineering world, many interesting mathematical techniques have only a limited impact because there are fewer technologies available to wrap these techniques up so they can impact non-expert users. The first step in connecting engineering and software technologies is understanding the role of technology standards in streamlining the development and deployment process. The next step is identifying applications where these technologies can have a significant impact on the the customers of engineered products. Along the way, we need to consider how to educate engineers, mathematicians and scientists about the possibilities that these technologies present and how to leverage them. This talk will discuss these issues and demonstrate examples of how engineering standards combined with cutting edge software technologies can help bridge the gap allowing engineers and mathematicians to have a greater impact on engineering product development and, ultimately, consumers. Specific topics will include mathematical models of products, cloud computing technologies and user experience in web-based engineering applications.

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MS43

Introduction and Overview of Modelica

Modelica is a declarative, equation based, object oriented language for the physics-based modeling of large scale engineering systems. Modelica is unique in being a vendor-neutral and widely accepted standard to describe such cyber-physical systems as the composition of Differential-Algebraic Equations (DAE) to describe the system physics and the software to control such systems. For the software part, several models of computation can be expressed in Modelica: signal oriented modeling, state machines, and synchronous declarative descriptions can all be expressed within the scope of Modelica. This combination makes Modelica useful through all phases of model based engineering, from the early phases of system design to the verification of the control software, and even reaching into system operation, where Modelica based models are used for non-linear model predictive control of complex and safety-critical plants. This talk will give an introduction to various aspects of Modelica from the perspective of applied mathematics and introduce how high-level Modelica code is transformed in several of the Modelica compilers to a range of numerical algorithms that are then used to analyze engineering design problems. In particular we will look at the transformation of Modelica code into hybrid DAE systems and to NLPs for solving optimal control problems.

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MS43

Modelica for Building and Community Energy Systems

Building energy and control systems can be represented by systems of coupled stiff differential equations, algebraic equations and discrete equations. These equations couple models from multiple physical domains. We will present how these systems can be modeled using the equation-based, object-oriented Modelica language. We discuss numerical challenges and opportunities to use such models for analysis that is outside the capabilities of conventional building simulation programs. The talk closes with an overview of the international project "new generation computational tools for building and community energy systems based on the Modelica and Functional Mockup Interface standards". This project is a collaboration among 16 countries under the Energy in Buildings and Communities Programme of the International Energy Agency.

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MS44

Dynamics Constrained Optimization of Power Grid Using Adjoint Sensitivity Analysis

We present a DAE-constrained optimization problem for the electric power grid where the steady state operating point has path constraints on the trajectory when the power grid is subjected to severe disturbances. We use constraint aggregration and adjoint sensitivity approach for efficiently solving this optimal control problem. This talk discusses the problem formulation, solution approach, and the preliminary results obtained.

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MS44

Global Error Estimation for Differential Equations

Global error represents the actual discretization error resulting after solving a system of differential equations. I will focus on time-stepping methods for ordinary and differential algebraic equations. Calculating a posteriori errors is generally viewed as an expensive process, and therefore in practice only the (local) error from one step to the next is used to estimate the global errors. However, local error estimation is not always suitable and may lead to error underestimation. I will review several strategies for a posteriori error estimation and discuss new approaches that generalizes the classical strategies.

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MS44

Predicting the Future with Faster Than Real-Time Power System Dynamics Simulation

"Faster than real-time dynamics simulation" is a key goal of DOE's Advanced Modeling Grid program. IIT is leading a project to (eventually) predict complex, large-scale power system behavior based on real-time measurements. The team is leveraging computational and hardware advances (e.g., PETSc solvers, time-stepping algorithms, and multi-core processors) to increase speed. Furthermore, the team is integrating modeling advances (e.g., three-phase unbalanced models, protection system models) to improve accuracy. The ultimate goal is to avoid blackouts.

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MS44

Dynamic-Feature Extraction, Attribution and Reconstruction (dear) Method for Power System Model Redution

This paper presents a method of deriving the reduced dynamic model of power systems based on dynamic response measurements. The method consists of three steps, namely dynamic-feature extraction, attribution, and reconstruction (DEAR), and results in a quasi-nonlinear reduced model of the original system. The network topology is unchanged. Tests on several IEEE standard systems show that the proposed method yields better reduction ratio and response errors than the traditional coherency based reduction methods.

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MS45

Improved Multilevel Monte Carlo for High Performance Computing

Since models at extreme scales may have high dimensional random space, it is important to continue the development of dimension-independent methods of uncertainty quantification. Here we accelerate MLMC for PDEs by using a FEM iterative solver that improves the initial guess during sampling. By using previous samples to build an interpolant that predicts the solution value at subsequent sample points, we can greatly reduce the number of iterations per MC sample. Implementation on GPU.

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MS45

A Multilevel Stochastic Collocation Methods for SPDEs

Multilevel methods for SPDEs seek to decrease computational complexity by balancing spatial and stochastic discretization errors. Multilevel techniques have been successfully applied to Monte Carlo methods (MLMC), but can be extended to accelerate stochastic collocation (SC) approximations. In this talk, we present convergence and complexity analysis of a multilevel SC (MLSC) method, demonstrating its advantages compared to standard single-level approximations, and highlighting conditions under which a sparse grid MLSC approach is preferable to MLMC.

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MS45

A Comparison of Algebraic Multigrid Preconditioning Approaches for Sampling-Based Uncertainty Propagation on Advanced Computing Architectures

Algebraic multigrid (AMG) methods are known to be effective, scalable preconditioners for linear systems arising in various application areas. Sampling-based uncertainty propagation methods provide an opportunity to extend such techniques to what are essentially groups of closely coupled systems. We compare AMG approaches in the context of ensemble propagation on advanced architectures, where sampling rearrangement has occurred in order to improve access and parallelism. Examples will be given using the Trilinos solver framework.

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MS45

Calibration of a Computer Model with Functional Inputs

We investigate the use of specialized experimental data to find Bayesian estimates of a functional parameter in a model of the system. Ideas are illustrated using a case study on the action potential of ventricular myocytes.

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MS46

Overview of High-Performance Algorithms for Functions of Matrices

In this talk I will present an overview of recent developments in high performance algorithms for matrix functions, with a focus on topics not covered by the subsequent talks in this minisymposium. I will discuss a selection of recent algorithms and results on condition estimation, the action of matrix functions on large, sparse matrices, and the implementation and testing of matrix function algorithms. I will also discuss some of the open problems and challenges involved in developing high-performance algorithms for matrix functions.

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MS46

Efficient and Stable Arnoldi Restarts for Matrix Functions Based on Quadrature

Arnoldi's method is a popular tool for approximating $f(A)b$, the action of a function f of a large sparse matrix A onto a vector b. The practical applicability of this method is limited by the storage requirements of the Arnoldi basis. We will discuss a new restarting technique based on quadrature which removes this limitation and is more stable and efficient than previously proposed restarting techniques. The new technique is applicable for a large class of functions f, including the so-called Stieltjes functions and the exponential function, both of which have applications in complex network analysis. Our method is applicable for functions of Hermitian and non-Hermitian matrices, requires no a-priori spectral information, and runs with essentially constant computational work per restart cycle.

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MS46

Exponential Iterative Methods of Runge-Kutta-type (EPIRK): Construction, Analysis and Software

Exponential integrators have recently emerged as an efficient alternative to the explicit and implicit methods for time integration of large stiff systems of differential equations. A distinct feature of these techniques is that the approximation of the solution uses exponential and exponential-like functions of the Jacobian or the matrices corresponding to the stiff linear part of the problem. Exponential integrators possess better stability properties compared to explicit methods and can require fewer calculations per time step then implicit schemes. We introduce a new class of Exponential Propagation Iterative methods of Runge-Kutta type (EPIRK). These schemes are designed to offer computational savings and allow construction of very efficient schemes compared to other exponential and implicit methods. We describe three different types of EPIRK methods - the unsplit, the split and the hybrid EPIRK schemes - as well as discuss a new type of implicit-exponential (IMEXP) methods. Both the classical and stiff order conditions for EPIRK integrators will be discussed and we will present a new software package EPIC (Exponential Propagation Integrators Collection) which implements most efficient of these methods for serial and parallel computational platforms.

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MS46

Blocked Algorithms for the Matrix Sign Function

The talk will describe two different blocked (partitioned) algorithms for the matrix sign functions. These algorithms offer improved performance over Higham's adaptation of the Schur-Parlett method for this problem. The improved performance is a result of reduced communication (fewer cache misses or less inter-processor communication). One variant uses existing efficient building blocks but requires the reordering of the Schur form, while the others has more overhead in the inner loop, but can utilize any ordering of the eigenvalues.

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MS47

Gradient Discretization of Hybrid Dimensional Two-Phase Darcy Flows in Fractured Porous Media

We present a gradient discretization, including a large family of schemes, in a case of a two-phase Darcy flow in discrete fracture networks (DFN) . We consider the asymptotic model for which the fractures are represented as interfaces of codimension one immersed in the matrix domain with continuous pressures at the matrix fracture interface. The convergence is proved under the assumption that the relative permeabilities are bounded from zero but cover the discontinuous capillary pressures. The numerical tests

are performed on the 3D fracture networks using Hybrid Finite Volume and the novel Vertex Approximate Gradient (VAG) discretizations. Compared with Control Volume Finite Element (CVFE) approaches, the VAG scheme has the advantage to avoid the mixing of the fracture and matrix rocktypes, while keeping the low cost of a nodal discretization on unstructured meshes. The efficiency of VAG scheme is shown in the case of a high permeability contrast between fracture network and matrix.

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MS47

A Double-Layer Reduced Model for Flow in Fault Zones Using Hybrid Finite Volume Schemes

We consider single-phase flows for subsurface porous media with faults, the latter along which the surrounding domain on one side of the fault has slipped with respect to that on the other. The fault width being smaller by several orders of magnitude than other characteristic sizes, we propose a hybrid finite volume method based on a double-layer, reduced model. We allow non-matching grids along the faults. Numerical and theoretical results are shown.

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MS47

Controlling Uncertainty in Fractured Porous Media Flow

We consider the dynamics of multiphase flow in heterogeneous porous media with randomly located interfaces. In the deterministic case the modeling of such systems requires the usage of nonlinear discontinuous flow functions. Based on the capillarity-free fractional flow formulation for two-phase flow, a hybrid stochastic Galerkin finite volume method (HSG-FV) is presented. The method accounts for the spatially random change of the mobilities and is particularly well-suited for parallel computations.

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MS47

A Fracture Indicator to Identify Fractures in Porous Media

We study the identification of fractures in porous media. The problem is formulated as a least squares minimization of a function evaluating the misfit between a measured pressure and a pressure calculated using a particular reduced discrete model for flow in porous media with fractures. Inspired by the idea of refinement indicators, we develop fracture indicators to search for fractures as well as their hydraulic conductivities through an iterative process.

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MS48

Learning Hierarchical Invariant Spatio-Temporal Features for Human Action and Activity Recognition

We propose a neural-network based learning scheme which computes a manifold in a bag of spatio-temporal features through regression based modeling. The action class models are designed to be independent of time without the need for sequence length normalization and initialization of states. Using the bag of spatio-temporal features as a time series data, a time-independent orthogonal basis is computed where a low-dimensional manifold is learned. Experimental results prove its efficiency on public data sets.

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MS48

An Inverse Kinematic Approach Using Groebner Basis Theory Applied to Gait Analysis of the Lower Extremity Joint Angles

This research highlights the results obtained from an experimental study of the lower limbs of a human gait cycle to extract and identify gait signatures. This biometric analysis was carried out by capturing the gait cycles in a normal and load bearing gait, using modalities such as passive infrared and passive optical. The challenge of this study is to distinguish between normal and abnormal gait signatures due to a concealed load on the lower body.

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MS48

Game-Theoretic and Reliability Methods in Counterterrorism and Security

The routine application of reliability analysis is not adequate in the security domain. Protecting against intentional attacks is fundamentally different from protecting against accidents or acts of nature. In particular, an intelligent and adaptable adversary may adopt a different offensive strategy to circumvent or disable protective security measures. Game theory provides a way of taking this into account. Thus, security and counter-terrorism require a combination of reliability analysis and game theory.

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MS48

Biomechanical Analysis of Pack Load Influence on Gait Signatures Derived from Grobner Basis Theory

This project examines kinematic gait patterns as predictors of the influence associated with individuals carrying concealed weighted packs up to 20% of their body weight. An initial inverse dynamics approach combined with computational algebra provided lower limb joint angles during the stance phase of gait as measured from 12 human subjects during normal walking. This talk describes the additional biomechanical analysis of the joint angle data to produce kinetic and kinematic parameters further characterizing human motion

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MS49

Numerical Optimization Method for Simulation Based Optimal Design Problems

The numerical optimization of simulation based problem is an interdisciplinary area of study that includes the optimization with PDE constraints area in applied mathematics. The Finite Element Method to find the numerical solution of a PDE subject to third-type boundary conditions as the ones that model electromagnetic phenomena, adjoint and direct differentiation gradients, and proper orthogonal decomposition are some of some of the topics of interest that continue to develop optimal design of devices.

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MS49

A Characterization of the Reflected Quasipotential

Our purpose here is to characterize the reflected quasipotential in terms of a first-order Hamilton-Jacobi equation. Because it is continuous but not differentiable in general the characterization will be in terms of viscosity solutions. Using conventional dynamic programming ideas, along with a complementarity problem formulation of the effect of the Skorokhod map on absolutely continuous paths, we will derive necessary conditions in the form of viscosity-sense boundary conditions.

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MS49

Analysis of Finite Difference Schemes for Diffusion in Spheres with Variable Diffusivity

Three finite difference schemes are compared for discretizing the spatial derivatives of the diffusion equation in spherical coordinates for the general case of variable diffusivity, D. Five diffusivity cases are considered: 1) constant D, 2) time-dependent D, 3) spatially-dependent D, 4) concentration-dependent D, and 5) implicitly time-dependent and spatially-dependent D. The results point to one of the schemes as the preferred finite difference method for numerically solving the diffusion equation in spheres with variable diffusivity.

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MS49

Analysis of Si Models with Multiple Interacting Populations Using Subpopulations with Forcing Terms

As a system of differential equations describing an epidemiological system becomes large with multiple connections between subpopulations, the expressions for reproductive numbers and endemic equilibria become algebraically complicated, which makes drawing conclusions based on biological parameters difficult. We present a new method which deconstructs the larger system into smaller subsystems, captures the bridges between the smaller systems as external forces, and bounds the reproductive numbers of the full system in terms of reproductive numbers of the smaller systems, which are algebraically tractable. This method also allows us to analyze the size of the endemic equilibria.

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MS50

Krylov Subspace Methods for Solving Singular Linear Systems or Least-Squares Problems

GMRES (Saad and Schultz 1986) is a famed generalized minimal-residual method for solving nonsingular unsymmetric or non-Hermitian linear systems. It may suffer non-benign breakdown on nearly singular systems (Brown and Walker 1997). When working, the solver returns only a least-squares solution for a singular problem (Reichel and Ye 2005). We present GMRES-QLP and GMRES-URV, both successful revamps of GMRES, for returning the unique pseudoinverse solutions of (nearly) singular linear systems or linear least-squares problems. On nonsingular problems, they are numerically more stable than GMRES. In any case, users do not need to know a priori whether the systems are singular, ill-conditioned, or incompatible; the solvers constructively reveal such properties. The solvers leverage the QLP and URV decompositions (Stewart 1998 and 1999) to reveal the rank of the Hessenberg matrix from the Arnoldi process, incurring only minor additional computational cost in comparison to GMRES. We present extensive numerical experiments to demonstrate the scalability and robustness of the solver, with or without preconditioners or restart.

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MS50

Probabilistic Bounds for Randomized Preconditioner for a Krylov Least Squares Solver

The Blendenpik algorithm by Avron, Maymounkov and Toledo solves least squares problems $\min ||Ax-b||$ for $m \times n$ matrices A with $rank(A) = n$, by computing a randomized preconditioner and applying the Krylov method LSQR to the preconditioned matrix. The preconditioner is computed by randomly sampling rows from A. We present probabilistic bounds for the condition number of the preconditioned matrix, when rows are sampled with replacement, and the sampling probabilities are uniform or based on leverage scores. Our bounds are derived from singular value bounds for a Monte Carlo matrix multiplication algorithm for computing the cross product AA'. For uniform sampling, the bounds imply that the number of sampled rows can be as much as 30 percent lower than existing bounds. For leverage-score based sampling, our bounds imply that the number of sampled rows must at least be a multiple of $n * ln(n)$. This is joint work with John Holodnak.

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MS50

IDR-CGS-BiCGSTAB-IDR(s) - a Case of Serendipity

In about 1976, the author was preparing a renovation of an elementary course on numerical analysis in Delft University. In relation to the problem of solving a single nonlinear equation iteratively, he wondered whether the so-called 'secant method' could be generalized to systems of N nonlinear equations with N unknowns, just for showing the students that there is something behind the horizon. Before starting to read everything on the subject, the author always tries to think about it unbiased, and so he started with, probably, re-inventing the wheel. Had he seen the book by Ortega and Rheinboldt at that time, CGS, BiCGSTAB and IDR(s) probably wouldn't exist today. Actually a new wheel was discovered, that appeared to be useful in the machinery of solving large sparse nonsymmetric *linear* systems. The first application of the new wheel was called IDR − Induced Dimension Reduction. Afterwards, CGS − Conjugate Gradients Squared − was developed as an 'improvement' of IDR, and also for other reasons. After CGS, in cooperation with Henk van der Vorst, (Bi-)CGStab was constructed, followed by a lot of other methods of this kind, developed by others. This went on until about 10 years ago. In this short presentation a reconstruction will be given of the strange history of these so-called 'Lanczos-type Product Methods'. It will be explained why this 'sleeping theory' woke up just after the author's retirement in 2006, resulting in a brand new family of methods: IDR(s). History is a continuing story, therefore some recently established features of IDR(s) will be mentioned.

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MS50

Multiple Preconditioners for GMRES

We propose a variant of GMRES which we call MPGMRES, whereby multiple (two or more) preconditioners are applied simultaneously, while maintaining minimal residual optimality properties. To accomplish this, a block version of Flexible GMRES is used, but instead of considering blocks starting with multiple right hand sides, we start with the initial residual and grow the space by applying each of the preconditioners to all current search directions and minimizing the residual norm over the resulting larger subspace. To alleviate the difficulty of rapidly increasing storage requirements and make the method practical, we further propose a selective algorithm that uses limited memory, and show theoretically and experimentally that this approach is highly effective. Convergence bounds for a special case are presented. Numerical results for problems in domain decomposition, PDE-constrained optimization, and fluid flow problems are presented, illustrating the viability and the potential of the proposed method. This is joint work with Chen Greif and Tyrone Rees.

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MS51

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS51

Analysis of the Volume-Constrained Peridynamic Navier Equation of Linear Elasticity

Well-posedness results for the state-based peridynamic nonlocal continuum model of solid mechanics are established with the help of a nonlocal vector calculus. The peridynamic strain energy density for an elastic constitutively linear anisotropic heterogeneous solid is expressed in terms of the field operators of that calculus, after which a variational principle for the equilibrium state is defined. The peridynamic Navier equilibrium equation is then derived as the first-order necessary conditions and are shown to reduce, for the case of homogeneous materials, to the classical Navier equation as the extent of nonlocal interactions vanishes. Using standard results, well-posedness is also established for the time-dependent peridynamic equation of motion.

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MS51

Is Dynamic Fracture at the Macroscale a Distinguished Limit of Unstable Nonlocal Bond Models?

We investigate a new class of models for solving problems of free crack propagation described by the peridynamic formulation. In the peridynamic formulation material points interact through short-range forces acting over a prescribed horizon. The formulation allows for discontinuous deformations and free propagation of cracks. We upscale the peridynamic model, passing to a small horizon limit, to find that the macroscopic evolution corresponds to the simultaneous evolution of the fracture surface and the linear elastic displacement away from the crack set. This provides a new connection between the dynamics of nonlocal short-range forces acting at the microscale to a brittle fracture evolution at the macroscale.

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MS51

Peridynamics as a Multiscale Method

Abstract not available at time of publication.

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MS52

Rigorous Computations for Nonlinear PDEs: An Introduction

Abstract not available at time of publication.

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MS52

Computer-Assisted Existence and Multiplicity Proofs for Semilinear Elliptic Boundary Value Problems

Abstract not available at time of publication.

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MS52

Rigorous Computation of Connecting Orbits

Abstract not available at time of publication.

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MS52

Rigourous Computation of a Bifurcation Diagram for the Ohta-Kawasaki Model

The Ohta-Kawasaki, or non-local Cahn-Hilliard, model is a simple description of energy-driven pattern formation with competing short- and long-range effects. One of the fundamental problems in this area is to identify which patterns have lowest energy in which regions of parameter space. We address this problem by finding the curves along which different solutions have the same energy. We use methods from rigourous computing to prove the existence of such curves and to get bounds between our discrete numerical approximations and the true infinite-dimensional solutions. Results from both two and three dimensions will be presented and discussed. This is joint work with JB van den Berg.

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MS54

The Exponential Formula for The Wasserstein Metric

Many evolutionary partial differential equations may be rewritten as the gradient flow of an energy functional, a perspective which can provide useful estimates concerning the behavior of solutions. The notion of gradient flow requires both the specification of an energy functional and a metric with respect to which the gradient is taken. In particular, much recent work has considered gradient flow in the Wasserstein metric. Given the formal nature of the gradient in this setting, a useful technique for constructing solutions to the gradient flow and studying their stability is to consider the "discrete gradient flow", a time discretization of the gradient flow problem analogous to the implicit Euler method in Euclidean space. In this talk, I will present a new proof that the discrete gradient flow converges to the continuous time gradient flow inspired by Crandall and Liggett's result in the Banach space case. Along the way, I will discuss theorems of independent interest concerning transport metrics.

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MS54

A Finite-Volume Method for Nonlinear Nonlocal Equations with a Gradient Flow Structure

We consider a finite volume method for the general equation

$$\rho_t = \nabla \cdot \Big[\rho \nabla \Big(H'(\rho) + V(\mathbf{x}) + W * \rho\Big)\Big], \quad \mathbf{x} \in \mathbf{R}^d$$

with the density of internal energy $H(\rho)$, the confinement potential $V(\mathbf{x})$ and the interactional potentail $W(\mathbf{x})$. A large variety of equations arises from physical or biological models can be written in this general form, and many important theoretical advances like optimal transportations are developed in certain special cases. The finite method is carefully designed to preserve the non-negativity of the solutions, and the total energy

$$E(\rho) = \int_{\mathbf{R}^d} H(\rho)\, d\mathbf{x} + \int_{\mathbf{R}^d} V(\mathbf{x})\rho(\mathbf{x})\, d\mathbf{x} + \frac{1}{2}\int_{\mathbf{R}^d}\int_{\mathbf{R}^d} W(\mathbf{x}-\mathbf{y})\rho(\mathbf{x})\rho(\mathbf{y})\, d\mathbf{x}\, d\mathbf{y}$$

is shown to be non-increasing in the semi-discrete form. We demostrate the effectiveness of this method with many examples, and show that it can be used to perform a numerical study of other unknown equations of similar types.

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MS54

Numerical Methods for the Fractional Laplacian

The fractional Laplacian is the seminal example of a nonlocal diffusion operator. Nonlocal diffusions are increasingly popular, and the fractional Laplacian is the prototypical model. Recent work by analysts including Caffarelli and Silvestre, among others, has studies nonlinear equations involving this operator, starting with the obstacle problem. But it solving even the one dimensional linear Fractional Laplacian equation on a bounded domain is a challenge which has not yet been addressed. It might appear that it should be quite simple to build schemes for the fractional Laplacian. For example the work of Valdinoci suggests that convolution kernels with the right decay will converge. The difficulty turns out to be accuracy: building even a first order accurate discretization is a challenge. The operator can be defined (and, in simple situations, approximated) using its Fourier symbol, which is multiplication by a power. However, when bounded domains are involved, the Fourier method is not as practical. The operator can also be represented as a singular integral: our method comes from a careful discretization of the singular integral. We apply rigorous numerical analysis methodology to the study of the fractional Laplacian. We derive a finite difference/quadrature method, and establish accuracy, a proof of convergence, careful truncation of the operator outside the computational domain, and numerical validation against exact solutions. Our method is compared favorably against existing methods, which do not have a rigorous foundation. We also apply the method to solve the obstacle problem.

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MS54

Error Estimates for Approximations to Fully Nonlinear PDE

We discuss error estimates for finite difference approximations to nonlinear elliptic and parabolic PDE. In particular, we highlight the relationship between error estimates and the regularity of solutions of the original equation. We present some recent progress and applications.

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MS55

Active Nano-Rod Dispersions

Within the large space of fluids that behave nonlinearly, we consider a niche fluid system between liquid crystals and active micro scale swimmers: active nano scale rod dispersions. We first highlight physical and biological systems that motivate our modeling, analysis, and simulations, and then take liberty to explore the models for rich phenomena that are reminiscent of behavior in either liquid crystals or bacterial suspensions.

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MS55

Physiological Boundary Conditions for Hemodynamics

A common goal in computational hemodynamics is the prediction of local blood flow downstream from stem arteries in which measurements are available. Due to computational complexity and uncertainties about the geometry and topology of the vasculature, such calculations are typically performed in a relatively small number of contiguous vessels. At the downstream edge of the computational domain, outflow boundary conditions have to be imposed. Choices of parameter values and type of conditions strongly impact the results, putting in question the significance of the entire modeling endeavor. We will discuss a new type of outflow boundary conditions allowing for a reduced reliance on calibration which is a major obstacle toward reliable patient specific simulations. Our approach allows the computation of the impedance of tiered structured vascular trees. It extends previous work from periodic to generic transient flows and relies on Laplace transforms and convolution quadratures. Joint work with Will Cousins (MIT) and Daniel Tartakovsky (UCSD)

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MS55

Two-Fluid Flow in a Capillary Tube

A phase field model for two-phase flow in a capillary tube, developed by Cueto-Felgueroso and Juanes, results in a PDE with higher-order terms. We find traveling wave solutions of the PDE and determine a bound on parameters to obtain physically relevant solutions. We observe that the traveling wave height decreases monotonically with capillary number. Finite difference simulations of the injection of a gas finger into water show a traveling wave advancing ahead of a rarefaction, leaving a plateau region of fluid adjacent to the tube wall. The residual thickness of this region was measured in experiments by G.I. Taylor in his famous 1961 paper. We find agreement between the traveling wave heights and the plateaus seen in the PDE simulations, and the results also compare favorably with the residual fluid thickness observed in the experiments. This is joint work with Rachel Levy, Ruben Juanes, and Luis Cueto-Felgueroso.

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MS55

A Saddle-Point Formulation And Finite Element Method For The Stefan Problem With Surface Tension

A dual formulation is proposed for the Stefan problem with surface tension (Gibbs-Thomson law). The method uses a mixed form of the heat equation in the solid and liquid domains, and imposes the interface motion law (on the solid-liquid interface) as a constraint. Well-posedness of the time semi-discrete and fully discrete (finite element) formulations is proved in 3-D, as well as an a priori bound, conservation law, and error estimates. Simulations are presented in 2-D.

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MS56

Mechanics and Evolution in Bacterial Biofilms

Bacteria frequently occupy densely populated surface-bound communities, termed biofilms. Biofilms behave like viscoelastic fluids at the macroscopic level. It is largely unknown how bacteria organize their behavior inside biofilms, and how biofilms behave in natural environments. In this talk, I will focus on how biofilms solve a classical evolutionary theory problem, the public goods dilemma, and how fluid physics shapes the dynamics of biofilms in complex environments.

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MS56

Hydrodynamics Affects Ordering and Organization in Bacterial Suspensions

We explore the nature and causes of the spontaneous ordering and organization that emerges in bacterial suspensions under confinement. Using simulations that capture oriented cell-cell and cell-fluid interactions, we show that hydrodynamics is crucial in reproducing and explaining the phenomena observed in recent experiments using bacteria B. Subtilis. We give new insights into the microscopic arrangement of the bacteria, which are confirmed by new experiments.

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MS56

Active Suspensions in Confinement

Active particle suspensions, of which a bath of swimming bacteria is a paradigmatic example, are characterized by complex dynamics involving strong fluctuations and large-scale correlated motions. These motions, which result from the many-body interactions between particles, are biologically relevant as they impact mean particle transport, mixing and diffusion, with possible consequences for nutrient uptake and the spreading of bacterial infections. In this work, we use a combination of kinetic theory and numerical simulations to analyze these effects, with particular focus on confined suspensions. I will specifically discuss the transport and effective rheology of dilute to semi-dilute suspensions in pressure-driven channel flows, as well as the pattern formation and complex dynamics arising in active suspensions confined in a Hele-Shaw geometry.

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MS56

Effects of Micro-swimmer Locomotion in Peristaltic Pumping

Peristaltic pumping is a form of fluid transport along the length of a tube containing liquid when the tube undergoes a contraction wave. While much is known about the peristalsis of Newtonian liquids, complex ones have received limited attention. If the fluid inside such a peristaltic micro-pump contains motile micro-particles (such as bacteria), then the net transport and mixing are affected by the micro-swimmer collective motion. We present a new numerical method that couples the motion of many micro-swimmers, the pump and the fluid flow. We show that the type of swimmer affects not only the net transport but can be utilised for mixing passive material.

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MS57

Social Aggregation in Pea Aphids: Experimental Measurement and Random Walk Modeling

Biological aggregations are found across the natural world. An ongoing challenge in the mathematical modeling of aggregations is to strengthen the connection between models and biological data by quantifying the rules that individuals follow. We model aggregation of the pea aphid, *Acyrthosiphon pisum.* Specifically, we conduct experiments to track the motion of aphids walking in a featureless circular arena in order to deduce individual-level rules. We observe that aphids follow a correlated random walk whose parameters depend strongly on distance to an aphid's nearest neighbor. We propose a random walk model and demonstrate that it reproduces the salient features of the observed macroscopic patterns of movement.

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MS57

Trajectory Dynamics of Aquatic Kleptoparasitic Interactions

Predation is among the most common pressures leading to group formation in animals. Although predator-prey systems have been studied extensively at the population level, relatively little work has been done to specify the individual behavioral decisions in such interactions. Here, we study a rather unique instance of kleptoparasitic interactions, whereby seagulls attempt to 'rob' flocks of aquatic seaducks of their food obtained from underwater dives. By reconstructing individual trajectories of both kleptoparasite and prey, we analyze the evasion behavior of the seaducks.

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MS57

Collective Dynamics in Laboratory Insect Swarms

Aggregations of social animals, think bird flocks or swarms of insects, are beautiful, natural examples of self-organized behavior far from equilibrium. Many models have been proposed to describe these systems, including agent-based models that specify social forces between individuals. We discuss measurements of laboratory midge swarms in the context of model assessment. In particular, we focus on the question of the small-number limit: how large must the population be before collective properties emerge?

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MS57

Oscillatory Patch Formations from Social Foraging

Dynamics of resource patches and foragers have been shown to exhibit pattern formations. Simple taxis of foragers towards randomly moving prey cannot lead to spontaneous formation of patchy environments. However, social interactions among foragers, specifically taxis in producer-scrounger group, can create novel spatiotemporal oscillatory patterns. I will also briefly discuss which of these behavior is more beneficial and how switching between strategies affect the resulting spatiotemporal patterns.

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MS58

Elastic Swimmer in Viscous Fluid: How to Swim Efficiently?

We use fully-coupled computer simulations to examine the low Re hydrodynamics of a self-propelling elastic swimmer. The swimmer is modelled as a thin elastic plate plunging at the root. The swimmer is free to move in the forward direction. We probe how swimming speed and efficiency depend on swimmer parameters. Our simulations reveal that the efficiency is maximized when the swimmer center of mass displacement is minimized. This regime reduces viscous losses, thereby enhancing the swimming efficiency.

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MS58

Mathematical Models for Microstructured Optical Fibre (MOF) Fabrication

We address various challenges arising in the fabrication of so-called microstructured optical fibres (MOFs) which guide light by virtue of a specially designed geometrical arrangement of channels running along their length. The fabrication involves placing a material (such as glass), heating it in a draw tower, and pulling it into a fibre so that the material is essentially a highly viscous (Stokes) fluid under an axial strain. The simultaneous effects of surface tension on the fibre/channel boundaries and the axial strain lead to deformations in the global fibre geometry that must be understood in order to arrive at the desired fibre state. This talk will describe recent progress in the mathematical modelling of this process [joint with P. Buchak and Y. Stokes].

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MS58

Accelerated Boundary Integral Simulations for Interactions of Drops and Solids in Micro-Fluidics

In micro-fluidic applications where the scales are small and viscous effects dominant, the Stokes equations are often applicable. Simulation methods can be developed based on boundary integral equations, which leads to discretizations of the boundaries of the domain only, reducing the number of unknowns. Two main challenges associated with boundary integral methods are to construct accurate quadrature methods for singular and nearly singular integrands, as well as to accelerate the solution of the dense linear systems that arise. For drops and solids in 2D, including also objects with sharp corners, we will discuss how to apply a general special quadrature approach to achieve highly accurate simulations also for very complicated settings. The simulations are accelerated with either the Fast Multipole method or a spectrally accurate FFT based Ewald method (for periodic problems). Simulation results for very challenging problems are presented.

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MS58

Self-Propulsion of An Inextensible Elastic Membrane in An Electric Field

In this work we illustrate a novel mechanism for self-propulsion of an inextensible elastic (lipid-bilayer) membrane subject to an electric field. In the lubrication framework, the dynamics of an inextensible elastic membrane is governed by a sixth order nonlinear partial differential equation with an integral constraint. Through numerical simulations we find (1) sloshing motion of the membrane, and (2) unit directional movement of the membrane, both in the direction transverse to the imposed electric field. We will also demonstrate how such movements of an elastic membrane can be further controlled by pattern electrodes and/or varying the temporal dependence of the external electric field. This work is a collaboration with Petia Vlahovska (Brown University). Y.-N. Young is partially supported by NSF grants DMS 1222550.

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MS59

Role of Network Topology in the Electromechanical Dynamics of Cascading Power Grid Failure

Recent work in analysis of cascading failure of electric power networks has sought to augment the quasi-steady state representations of prior literature with faster time scale electromechanical dynamics, and with threshold-driven relay action that disconnects network links upon overload. In these dynamic models, cascading failure appears as a sequence of transitions between locally stable equilibria, each corresponding to a partially degraded network structure, and with the most vulnerable paths of transition passing through saddle point unstable equilibria. This work will explore the role of network topology in predicting the location of these saddle exits in the state space, and the interplay of topology and relay threshold values in determining the disturbance energy that must be injected into the system to drive the state over such a saddle point.

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MS59

Centrality of Dynamical Graph Structures

We consider adapting well known graph centrality measures to the case of dynamic graphs or static graphs with dynamic forcing functions. For instance, we present the PageRank method on a static graph with time-varying teleportation and demonstrate a closed form analytical solution that involves complex valued teleportation parameter. We consider how these could be deployed for studying power systems and contingency analysis.

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MS59

Stochastic Graph Modeling of Power Grids

Graph-theoretic approaches have long been used for characterizing the topological structure of power grids. The central idea of such approaches is to use known algorithms for generating random graphs and then using graph-based metrics to match the characteristics with those from real-world power grid models, such as the Western and Eastern Interconnects. In our work, we are exploring several variants of the random geometric graph algorithm for the

purposes of generating synthetic models of the power grid. By exploiting the inherent hierarchical structure in voltage levels, we show that random geometric graph models can be used to generating synthetic power grids.

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MS59

Algorithms for Monitoring Oscillations in the Power Grid

Monitoring the oscillations in the power grid in real-time is an increasingly difficult challenge due to the large number of components. Additionally, large numbers of Phasor Measurement Units (PMUs) are being deployed to generate large-scale data on the state of the grid. Algorithms for computing a few singular values and vectors and updating these are critical components to monitor the oscillations. We describe efficient algorithms to compute and update the singular value decompositions in this context.

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MS60

RBF-FD for Mesoscale Nonhydrostatic Atmospheric Modeling

In applications of radial basis functions (RBFs) for fluid modeling, infinitely smooth RBFs have traditionally been used due to the spectral convergence properties. However, fluid flows in nature can exhibit complex features such that spectral accuracy cannot be realized on resolutions that are observable or practical. A novel approach for modeling with RBF-generated finite differences (RBF-FD) is presented by using polyharmonic spline RBFs together with high-order polynomials. The approach is tested on nonhydrostatic atmospheric flows.

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MS60

RBF-FD for Elastic Wave Propagation in Layered Media

Seismic exploration is used to map out hydrocarbon deposits. In forward modeling, substructures are assumed to be known, and the task is to simulate elastic wave propagation through the medium. Inversion programs then update substructure assumptions to reconcile the model response with actual measurements. We have found that RBF-FD spatial discretization offers outstanding accuracy and algebraic simplicity for modeling elastic wave propagation, especially in layered media with large numbers of irregularly curved interfaces.

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MS60

Application of the RBF-FD Method to Laminar Flame Propagation Problems

Premixed flame propagation is an important topic in combustion research with many applications in energy and safety. In this paper we apply the RBF Finite difference (RBF-FD) method to solve the equations describing laminar fame propagation in two-dimensional and three-dimensional ducts. We use stencils with a relatively large number of nodes in order to achieve high order accuracy. Finally, we apply this methodology to solve a simplified mathematical model describing flame propagation in a rotary engine microcombustor.

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MS60

Modeling Ocean Dynamics Using RBF-FD

RBFs have started to emerge as a powerful tool, not only for interpolation, but also for discretizing differential operators. Over the last few years, new approaches have been developed to bypass the method's well-known problems of stability and of large computational complexity. Such a new approach resulted in the RBF-FD method which enjoys high accuracy, has an intrinsic ability to represent complicated geometries in any dimension, still has a remarkable algorithmic simplicity, and leads to a sparse differentiation matrix. We will use this technique to solve the Navier-Stokes equations and discuss its potential as a high-order method for the modeling of oceanic phenomena.

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MS61

Electromagnetic Wave Propagation in Random Waveguides

I will describe an analysis of electromagnetic wave propagation in waveguides filled with heterogeneous media, modeled by a random electric permeability. The waves are trapped by perfectly conducting boundaries and the goal of the analysis is to quantify the long range net scattering effects of the random medium. The result is a detailed characterization of the transport of energy, the loss of coherence and the depolarization of the waves due to scattering. I will give some numerical illustrations and will compare the theory with that of scalar (acoustic) wave propagation in random waveguides.

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MS61

Homogenization of Interfaces Moving with Spatio-temporal Periodic Velocity

Abstract not available at time of publication.

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MS61

Imaging Multiply Scattering Point Targets Using Sparsity Promoting Optimization

We study active array imaging of small but strong scatterers in homogeneous media when multiple scattering between them is important. We discuss a non-iterative approach that solves the imaging problem in two steps using sparsity promoting optimization. We analize the uniqueness and stability of this imaging method using both single and multiple illuminations. To improve its robustness and the resolution of the images we also discuss the use of optimal illuminations. This is join work with Anwei Chai and George Papanicolaou.

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MS61

Correlation Based Imaging and Applications

Abstract not available at time of publication.

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MS62

Numerical Assessment of the Risk of Rock Damage in the Vicinity of Salt Caverns for the Storage of Gaseous Matter at Cyclic Operation Conditions

Abstract not available at time of publication.

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MS62

Numerical Simulation of Deformation and Flow in Fractured, Poroelastic Materials

We introduce a coupled system of PDEs for the modeling of the fluid-fluid and fluid-solid interaction in a fractured, poroelastic material. The fluid flow in the fracture is modeled by a lower-dimensional equation, which interacts with the surrounding rock matrix and the fluid it contains. To determine the mechanical and hydrological equilibrium of the system numerically, we combine an XFEM discretization for the rock matrix deformation and pore pressure with a lower-dimensional grid for the fracture. The resulting coupled discrete problem is solved using a substructuring method.

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MS62

Fracture Propagation in Porous Media Using Isogeometric Analysis

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MS62

Coupling Fluid Flow with Stresses Induced by Fracture Deformation in Discrete Fracture Networks

Fluid flow in fractures can cause deformation, but induced stresses can be challenging to implement in numerical models, especially in large DFNs. I will describe CFRAC, a simulator I developed that implicitly couples fluid flow, fracture deformation, transmissivity evolution, friction evolution, and fracture propagation, and is efficient enough to simulate (2D) networks with thousands of fractures. I will describe model behaviors that emerge from interactions between processes and which give insight into complex physical systems.

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MS63

Learning the Association of Multiple Inputs in Recurrent Networks

In spite of the many discoveries made in neuroscience, the mechanism by which memories are formed is still unclear. To better understand how some disorders of the brain arise, it is necessary to improve our knowledge of memory formation in the brain. With the aid of a biological experiment, an artificial neural network is developed to provide insight into how information is stored and recalled. In particular, the bi- conditional association of distinct spatial and non-spatial information is examined using computational model. This model is based on a combination of feedforward and recurrent neural networks and a biologically-inspired spike time dependent plasticity learning rule. The ability of the computational model to store and recall the bi-conditional object-space association task through reward-modulated plastic synapses is numerically investigated.

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MS63

Mechanistic Models of Retinitis Pigmentosa

In this talk we will give a brief overview of our work as it pertains to Retinitis Pigmentosa (RP). With mathematics and computer (in silico) experiments, we explore the experimentally observed photoreceptor death and rescue in the progression of RP. Using mechanistic mathematical models of photoreceptor interactions in the presence of RP we (1) trace the evolution of RP from one stage to another in each main subtype, (2) capture the rod and cone wave deaths, and (3) explore various treatment regiments via RdCVF. Our work highlights the delicate balance between the availability of nutrients and the rates of shedding and renewal of photoreceptors needed for a normal functioning retina and to halt the progression of RP. This work provides a framework for future physiological investigations potentially leading to long-term targeted multi-faceted interventions and therapies dependent on the particular stage and subtype of RP under consideration.

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MS63

Dynamics and Control of An Invasive Species: The Case of the Rasberry Crazy Ant Colonies

This project is motivated by the costs related with the documented risks of the introduction of non-native invasive species of plants, animals, or pathogens associated with travel and international trade. Such invasive species often have no natural enemies in their new regions. The spatiotemporal dynamics related to the invasion/spread of Nylanderia fulva, commonly known as the Rasberry crazy ant, are explored via the use of models that focus on the reproduction of ant colonies. A Cellular Automaton (CA) simulates the spatially explicit spread of ants on a grid. The impact of local spatial correlations on the dynamics of invasion is investigated numerically and analytically with the aid of a Mean Field (MF) model and a Pair Approximation (PA) model, the latter of which accounts for adjacent cell level eects. The PA model approach considers the limited mobility range of N. fulva, that is, the grid cell dynamics are not strongly inuenced by non-adjacent cells. The model determines the rate of growth of colonies of N. fulva under distinct cell spatial architecture. Numerical results and qualitative conclusions on the spread and control of this invasive ant species are discussed.

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MS63

Qualitative Inverse Problems Using Bifurcation Analysis in the Recurrent Neural Network Model

We develop a framework for determining when there is bistability and multistability in the expression states of systems described by the recurrent neural network (RNN) model. Our results show that, although bistability can be generated with autoregulation, it is also the case that both autorepression or no autoregulation can yield bistability as long as a sigmoidal behavior is present. Additionally, our results suggest that allowing only a single connection when inferring a network may be a reason why parameter values in the inferred gene networks in the literature are not be realistic.

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MS64

Organism - Effects of Nonlinearities on Lamprey

Locomotion

The lamprey is a basal vertebrate and a model organism for neurophysiology and locomotion studies. Here a 2D, integrative, multi-scale model of the lamprey's anguilliform (eel-like) swimming is driven by neural activation and muscle kinematics coupled to body interactions with fluid surroundings. The fluid-structure interaction problem is solved numerically using an adaptive version of the immersed boundary method (IBAMR). Effects on swimming speed and cost by nonlinear dependencies associated with muscle force development are examined.

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MS64

The Breadth of Mathematical Modelling of Biological Systems: History and Opportunities

An overview of a number of established areas in mathematical biology, as well as more recent opportunities that have emerged, will be presented as an introduction to this session. In particular, the importance that nonlinearities often pose, both in terms of reflecting realistic biological dynamics and the mathematical challenges that arise in analyzing the resulting models, will be emphasized. Recent illustrations of integrative research in this area in which the mathematical sciences guide biological studies and experimental work and field data inform the modeling will be discussed.

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MS64

CellularNonlinear Models for Predicting Immune Response Mechanisms

Johne's disease, a persistent and slow progressing infection in ruminants such as cows and sheep is caused by Mycobacterium avium subspecies paratuberculosis (MAP) bacillus. Mycobacterial infections are associated with complex immune response mechanisms whose underlying biology is not clearly understood. Host immune response to MAP infection is associated with predominance of a cell mediated response in its early stages and a switch to the dominance of antibody response with concomitant disease progression. How the switch in immune response predominance occurs is not clearly known. In this study, we developed series nonlinear models to predict the underlying immune response mechanisms associated with MAP-bacteria shed in cattle feces. Immune response mechanisms are identified by fitting these models to immune response data and longitudinal fecal shedding patterns of experimentally infected cattle. Using statistical model selection methods, we were able to discriminate potential animal immune response mechanisms that can explain the variant shedding patterns for each infected animal. Our results suggest that there are specific variant immune response mechanisms that could be silent in other animals, however, these could be active in other animals, hence varying MAP shedding patterns and disease progression trends.

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MS64

Variability in Species Abundance Distributions from Nonlinear Stochastic Competition Models

Species abundance distributions (SADs) are metrics for ecological communities, or sets of similar species in an ecosystem. Using a nonlinear stochastic competition model, I will show that SADs of communities with neutral dynamics (demographic stochasticity and immigration) differ from those of communities with niches (clusters of similar species) arising under trait-based competition, and quantify the likelihood of being able to use this metric to distinguish between these two community types based on abundance data alone.

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MS65

Block Preconditioners for Saddle-Point Linear Systems

Symmetric indefinite 2×2 and 3×3 block matrices are featured prominently in the solutions of constrained optimization problems and partial differential equations with constraints. When the systems are large and sparse, modern iterative methods are often effective. For block-structured matrices it is often desirable to design block diagonal preconditioners. In this talk a few block preconditioning approaches are discussed. We focus on the case of a maximally rank deficient leading block, which gives rise to interesting algebraic properties that can be exploited in the design of preconditioners. The use of Schur complements and null space matrices is illustrated.

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MS65

Krylov Subspace Methods for Large Scale Matrix Equations

Given the square large matrices A, B, D, E and the matrix C of conforming dimensions, we consider the numerical solution of the linear matrix equation $A\mathbf{X}E + D\mathbf{X}B = C$ in the unknown matrix $\mathbf{X}$. These matrix equations are becoming a reliable tool in the numerical treatment of advanced mathematical models in engineering and scientific computing. Our aim is to provide an overview of the major algorithmic developments in projection methods based on

Krylov-type subspaces, that have taken place in the past few years.

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MS65

Krylov Subspaces and Dense Eigenvalue Problems

When we think of Krylov subspace methods, we normally think of large, sparse problems. It is not widely appreciated that Krylov subspace ideas are also applicable to dense linear algebra. In this talk, which is more pedagogy than research, we show how thinking about Krylov subspaces leads to a powerful algorithm for solving dense eigenvalue problems. Unfortunately the algorithm is not new; it was invented over 50 years ago by John Francis.

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MS65

Computing Singular Values of Large Matrices with an Inverse Free Preconditioned Krylov Subspace Method

We present an efficient algorithm for computing a few extreme (largest and smallest) singular values and corresponding singular vectors of a large sparse $m \times n$ matrix C. Our algorithm is based on reformulation of the singular value problem as an eigenvalue problem for $C^T C$ and, to address the clustering of singular values, we use an inverse-free preconditioned Krylov subspace method to accelerate convergence. We consider preconditioning that is based on robust incomplete factorizations and we discuss various implementation issues. Extensive numerical tests are presented to demonstrate efficiency and robustness of the new algorithm.

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MS66

Closure-based Algorithms for Simulation of Mesoscale Evolution of Large ODE Systems

We study a problem of designing efficient methods based on space-time averaging for simulation of mesoscale dynamics of large particle systems. Averaging produces exact mesoscale partial differential equations but they cannot be simulated without solving the underlying microscale system. To simulate these mesoscale equations independently, we consider several closure methods including regularized deconvolution closure and kinetic closure. We investigate the relationship between their accuracy and computational cost.

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MS66

Forward and Inverse Homogenization of Maxwell's Equations in Time Domain

The talk discusses a time domain problem for Maxwell's equations for a multiscale dispersive medium. Homogenization results in time-convolution equations with a memory kernel. We relate this kernel to the spectral measure of the local problem and use it to derive information about the microgeometry of the finely structured medium.

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MS66

On Reconstruction of Dynamic Permeability and Tortuosity of Poroelastic Materials

Dynamic permeability refers to the permeability of poroelastic media subjecting to oscillatory pressure gradient. It depends on both the frequency and the pore space geometry. The dynamic tortuosity is inversely related to the dynamic permeability and plays an important role in the mechanism of energy dissipation of waves through poroelastic materials. Numerically, dynamic tortuosity is the kernel in the memory term in the dissipation term for time domain wave equations; it is known to be associated with fractional derivative of order 1/2. In this talk, we will present our results on reconstructing the dynamic permeability as a function of frequency from partial data by utilizing its analytical properties when extending to the complex frequency plane. Using the relation between tortuosity and permeability, a set of quadratures are constructed for handling the memory term in the poroelastic wave equations.

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MS66

Kinetic Equation for Spatial Averages of Particle Dynamics

Abstract not available at time of publication.

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MS67

Symmetry and Bifurcations in First-order PDEs with Nonlocal Terms Modelling Animal Aggrega-

tion

Pattern formation in self-organised biological aggregation is a phenomenon that has been studied intensively over the past twenty years. I will present a class of models of animal aggregation in the form of two first-order hyperbolic partial differential equations on a one-dimensional domain with periodic boundary conditions, describing the motion of left and right moving individuals. The nonlinear terms appear using nonlocal social interaction terms for attraction, repulsion and alignment. This class of models has been introduced in the Ph.D thesis of R. Eftimie. In this talk, I will show that the equations are $\mathbf{O}(2)$ equivariant where the group $\mathbf{O}(2)$ is generated by space-translations and a reflection which interchanges left-moving individuals with right-moving individuals across the middle of the interval. I will discuss steady-states and their symmetry with a focus on homogeneous $\mathbf{O}(2)$ symmetric states and the existence of codimension two steady-state/steady-state, steady-state/Hopf and Hopf/Hopf bifurcation points. I will discuss how using existing symmetry-breaking bifurcation theory and new theoretical results, one can study the neighborhood of those bifurcation points and classify the patterns obtained. This is joint work with R. Eftimie (U. Dundee, Scotland).

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MS67

Network Symmetry and Binocular Rivalry Experiments

Hugh Wilson has proposed a class of models that treat higher-level decision making as a competition between patterns coded as levels of a set of attributes in an appropriately defined network. In this talk, I will propose that symmetry-breaking Hopf bifurcation from fusion states in suitably modified Wilson networks can be used in an algorithmic way to explain the surprising percepts that have been observed in a number of binocular rivalry experiments.

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MS67

Spontaneous Symmetry-Breaking in Neural Morphology

A developing neuron initially extends several protrusions which are similar in length, but selects a single one which elongates much longer than the others and becomes an axon. This morphological symmetry breaking is important for the neuron to form its input (dendrite) and output (axon) devices. In this talk, we introduce quantitative mathematical model of the neuronal symmetry breaking as a nonlinear dynamical system, and show how symmetry breaks by phase plane analysis.

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MS68

Mathematical Modelling of Wind Turbines

America is home to one of the largest and fastest growing wind markets in the world. In 2012 the United States wind power installations were more than 90% higher than in 2011. With the growing demand for installations, the need for mathematical modelling has become critical. In this talk, I will describe a simple model of a wind turbine and some of it's applications. Future lines of research will also be discussed.

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MS68

Well-Balanced Positivity Preserving Central-Upwind Scheme for the Shallow Water System with Friction Terms

Shallow water models are widely used to describe and study free-surface water flow. The friction terms will play a significant role when the depth of the water is very small. In this talk, we introduce shallow water equations with friction terms and a well-balanced central-upwind scheme that is capable of exactly preserving physically relevant steady states. The data in the numerical example correspond to the laboratory experiments designed to mimic the rain water drainage in urban areas.

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MS68

Membrane Deformation by Protein Inclusions

I will explore various models for the deformation of biomembranes by protein molecules which are embedded in or attached to the membrane, termed protein inclusions. Mathematically we focus on minimisation problems involving the Helfrich energy functional. Inclusions will be modelled by enforcing pointwise constraints on the membrane displacement or curvature. I will present results detailing the existence and behaviour of minimal energy states for some of these models.

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MS68

Modeling Feral Hogs in the Great Smoky Mountains National Park

Feral Hogs (Sus Scrofa) are an invasive species that have occupied the Great Smoky Mountains National Park since the early 1900s. Recent studies have revitalized interest in the pest and have produced useful data on vegetation, mast and harvest history. Using these data, a model with discrete time and space was formulated to represent the hog dynamics in the park. Management strategies and estimation of actual total population was investigated.

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MS68

Stochastic Diffusion Processes in Systems Biology

In cell biology many species are only present at very low copy numbers, therefore a deterministic description by partial differential equations often doesnt reproduce experimental results and a stochastic model is needed. We use a continuous-time discrete-space Markov process to simulate diffusion stochastically. To represent complex geometries accurately we discretize the cell into an unstructured mesh and compare the jump coefficients resulting from a finite element method and a first exit time approach.

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MS68

A Smoothing Trust Region Filter Algorithm for Nonsmooth Nonconvex Least Squares Problems

We propose a smoothing trust region filter algorithm for nonsmooth and nonconvex least squares problems with zero residual. We present convergence theorems of the proposed algorithm to a Clarke stationary point or a global minimizer of the objective function under certain conditions. Preliminary numerical experiments show the efficiency of the proposed algorithm for finding zeros of a system of polynomial equations with high degrees on the sphere and solving differential variational inequalities.

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MS69

Filtered Spectral Methods for Transport Problems

We analyze the behavior of filtered spectral approximations that are used in the angular discretization of radiative transport equations. Recently the filtering approach has been recast as a transport equation with modified scattering cross-section. We examine this modified equation, prove some basic convergence properties, and show some supporting numerical results.

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MS69

Hybrid Algorithms for Hybrid Computers: Kinetic-Continuum Models of Transport Phenomena

Recent developments in high-performance computing have led to a hybrid architecture composed of multicore CPUs and GPU coprocessors (e.g. ORNL Titan machine). In such architectures, a premium is placed on algorithms that require minimal communication between CPU/GPU nodes. We introduce a set of algorithms in this spirit based upon stochastic differential equation solvers for kinetic level models of transport phenomena, coupled with high-order finite element models of the continuum (homog-

enized) scale.

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MS69

Hydraulic Modeling for Quantum Absorption Calculation in Plasmonics Based on High-Order Spectral Element Discontinuous Galerkin Approach

I will discuss about recent development of spectral element discontinuous Galerkin (SEDG) schemes for solving local interactions between electrons and the light in plasmonic systems. The dispersive material properties of the system are described by a hydraulic model. This approach is formulated by coupling the macroscopic Maxwell equations with the equations of motion of the electron gas. The nonlocal polarization current induced by an external electromagnetic field is represented by a system of the first-order partial differential equations with an auxiliary ordinary differential equation. I will present efficient and stable SEDG algorithms with properly designed numerical fluxes, provided with stability analysis. We validate our computational results for nano sized metallic cylinders for the absorption cross sections and field distributions.

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MS69

Semi-Lagrangian Discontinuous Galerkin Schemes for the Relativistic Vlasov-Maxwell System

The Vlasov-Maxwell system describes the evolution of a collisionless plasma, represented through a probability density function (PDF) that self-interacts via the electromagnetic force. One of the main difficulties in numerically solving this system is the severe time-step restriction that arises from parts of the PDF associated with moderate-to-large velocities. The dominant approach in the plasma physics community is the so-called particle-in-cell method. The focus of the current work is on semi-Lagrangian methods. In particular, we develop a method based on high-order discontinuous Galerkin (DG) scheme in phase space, and an operator split, semi-Lagrangian method in time. The method is designed to be (1) high-order accurate, (2) mass conservative, and (3) positivity-preserving. The resulting scheme is applied to laser-plasma acceleration problems.

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MS70

Optimal Control of Free Boundary Problems with Surface Tension Effects

We will give a novel proof for the second order order sufficient conditions for an optimal control problem where the state system is composed of Laplace equation in the bulk and Young-Laplace on the free boundary. Next, we will discuss a novel analysis for a Stokes free boundary problem with surface tension effect. We will conclude with some recent results for the Navier-Stokes problem with slip boundary conditions.

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MS70

Numerical Investigations of Bouncing Jets

The Kaye effect is a fascinating phenomenon of a leaping shampoo stream which was first described by Alan Kaye in 1963 as a property of non-Newtonian fluid. It manifest itself when a thin stream of non-Newtonian fluid is poured into a dish of fluid. As pouring proceeds, a small stream of liquid occasionally leaps upward from the heap. We investigate numerically the impact of the experimental setting as well as the fluid rheology on the apparition of bouncing jets. In particular, we observe the importance of the creation of a thin lubricating layer of air between the jet and the rest of the liquid. The numerical method consists of a projection method coupled with a level-set formulation for the interface representation. Adaptive finite element methods are advocated to capture the different length scales inherent to this context.

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MS70

Splitting for Variable Density Flows

We show the equivalence between the so-called gauge Uzawa method and the pressure correction schemes in rotational form. Using this equivalence we show simpler stability proofs for known schemes and devise a new stable scheme for the approximation of incompressible flows with variable density. The main feature of the new method is that only involves constant, in time, matrices.

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MS70

Modeling Viscoelastic Networks in Stokes Flow

We present a simple method for modeling heterogeneous viscoelastic media at zero Reynolds number. The method can be extended to capture viscoelastic features as well as some other models. Linking rules for the network are based on linear viscoelastic models, then varying complexity allows the model to exhibit different kinds of behavior. A few rheology tests are used to analyze the mechanical properties of the model networks and the effects of input parameters on these properties.

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MS71

Interferometric Waveform Inversion: Geophysics Meets Spectral Graph Theory

In seismic and SAR imaging, fitting cross-correlations of wavefields rather than the wavefields themselves can result in improved robustness vis-a-vis model uncertainties. This approach however raises two challenges: (i) new spurious local minima may complicate the inversion, and (ii) one must find a good subset of cross-correlations to make the problem well-posed. I will explain how to address these two problems with lifting, semidefinite relaxation, and expander graphs. This mix of ideas has recently proved to be the right approach in other contexts as well, such as angular synchronization (Singer et al.) and phase retrieval (Candes et al.). Joint work with Vincent Jugnon.

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MS71

Inverse Born Series for the Radiative Transport Equation

We propose a direct reconstruction method for the inverse radiative transport problem that is based on inversion of the Born series. We characterize the convergence and approximation error of the method and illustrate its use in numerical simulations.

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MS71

Layered Media Scattering: Fokas Integral Equations and Boundary Perturbation Methods

In this talk we describe a class of Integral Equations to compute Dirichlet-Neumann operators for the Helmholtz equation on periodic domains inspired by the recent work of Fokas and collaborators on novel solution formulas for boundary value problems. These Integral Equations have a number of advantages over standard alternatives including: (i.) ease of implementation (high-order spectral accuracy is realized without sophisticated quadrature rules), (ii.) seamless enforcement of the quasiperiodic boundary conditions (no periodization of the fundamental solution, e.g. via Ewald summation, is required), and (iii.) reduced regularity requirements on the interface proles (derivatives of the deformations do not appear explicitly in the formulation). We show how these can be efficiently discretized and utilized in the simulation of scattering of linear acoustic waves by families of periodic layered media which arise in geoscience applications.

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MS71

Numerical Algorithms for Simultaneous Determination of Acoustic and Optical Coefficients in Photoacoustic Tomography

Photoacoustic tomography (PAT) aims at reconstructing physical properties of optically heterogeneous media from measured acoustic signals generated by the photoacoustic effect. Image reconstructions in PAT are usually done in a two-step process. In the first step, one solves an inverse wave propagation problem to recover the initial pressure field inside the media. In the second step, one solves an inverse diffusion/transport problem to recover optical properties, using the result of the first step as the data. This two-step procedure breaks down when the acoustic wave speed is also assumed unknown and to be reconstructed. We present here some numerical algorithms that solve the inverse wave and inverse diffusion problems simultaneously to image both optical and acoustic properties.

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MS72

Hydrodynamic Interaction of Swimming Microorganisms in Complex Fluids

The interaction of motile microorganisms, surrounding fluids and boundaries is of paramount importance in a variety of physical and environmental phenomena including the development of biofilms, colonization of microbes in viscoelastic mucus of human and animal bodies, bacterial aggregating in oceanic gels, and swimming of spermatozoa in female reproductive tract. In this study, we scrutinize the role of rheological properties of background fluids on the interaction of microorganisms with rigid surfaces.

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MS72

Swimming Through Heterogeneous Networks

I will present results for swimmers moving near similar-size microstructural heterogeneities. Spherical obstructions are used to deduce physical principles linking the swimmer flow field, forces on obstructions, and changes in swimming velocities. Then single rod-like obstructions are studied to deduce the effect of a network of filaments. The average and variance of the swimming speed reflect the density and orientation correlations of the microstructure, and hence swimming properties can be used as probes of microstructure.

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MS72

Mechanism of Microorganism Propulsion in Viscoelastic Fluids

Abstract not available at time of publication.

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MS72

Flagellar Locomotion in Viscoelastic and Anisotropic Environments

We will discuss recent investigations of helical and undulatory locomotion in viscoelastic (Oldroyd-B) and anisotropic (liquid crystal) fluids. Elastic and anisotropic effects can either enhance or retard a microorganism's swimming speed, and can even change the direction of swimming, depending on the body geometry and the fluid properties. Our findings connect studies showing situationally dependent enhancement or retardation of swimming speeds, and may help to clarify phenomena observed in a number of biological systems.

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MS73

The Response of the Lyapunov Exponent to External Perturbations

We present a new approach to predict the response of the largest Lyapunov exponent of a dynamical system to small external perturbations of different types. The connection between the external perturbation and the change in the largest Lyapunov exponent is approximately represented through the corresponding response operator, computed for the original unperturbed system. The theory for the response operator of the largest Lyapunov exponent is based on the well-known Fluctuation-Dissipation theorem. We also compute the response prediction for a simple model of chaotic nonlinear dynamics, and compare it against the actual response of the largest Lyapunov exponent computed by directly perturbing the system, for a simple constant forcing perturbation.

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MS73

Stochastic Mode-Reduction in Models with Conservative Fast Sub-Systems

We will consider application of the stochastic mode reduction to multi-scale models with deterministic energy-conserving fast sub-system. In particular, we consider the situation when the slow variables are driven stochastically and interact with the fast subsystem in an energy conserving fashion. Since there is energy exchange between the fast conservative sub-system and the slow variables, it is necessary to explicitly keep track of the energy of the fast sub-system. Therefore, we develop a new stochastic mode reduction process in this case by introducing energy of the fast subsystem as an additional hidden slow variable. We use several prototype models to illustrate the approach.

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MS73

Stochasticity in An Integrable System: Pulse Polarization Switching in An Active Optical Medium

Propagation of optical pulses through an active optical medium with two working levels, known as the Lambda-configuration, is described by an initial-boundary value problem for a set of completely integrable partial differential equations. If the initial conditions are prepared randomly, the resulting soliton solutions exhibit stochastic behavior, which can be described exactly in terms of probability-density functions and first- and last-passage time problems. The talk will present these soliton statistics.

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MS73

Dynamics of Ferromagnets

Driving nanomagnets by spin-polarized currents offers exciting prospects in magnetoelectronics, but the response of the magnets to such currents remains poorly understood, even more so with the addition of thermal noise. For a single domain ferromagnet, I will show that an averaged equation describing the diffusion of energy on a graph captures the low-damping dynamics of these systems. I will then present the problem of extending the analysis to spatially non-unifrom magnets, modeled by an infinite dimensional Hamiltonian systems, equivalently a non-linear wave equation with stochastic in space initial conditions.

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MS74

Data Analytics Throughout Undergraduate Math-

ematics

DATUM is an education/research program which trains freshman and sophomore students in the philosophy and tools of data analysis and modeling. The course, Introduction to Data Mathematics, introduces high-dimensional modeling, data analytics, and their use in applications. Requiring only basic calculus, it prepares students for summer research on real-world data analytics problems. It teaches data analytics methods along with a targeted examination of underlying high-dimensional mathematics including Euclidean geometry, matrix algebra, eigenvalues, and spectral decomposition.

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MS74

Research and Training in Computational and Data-Enabled Science and Engineering for Undergraduates in the Mathematical Sciences at NJIT

The NJIT EXTREEMS-QED program is designed to immerse undergraduates in courses and group research projects in the computational analysis of data and the modeling and simulation of complex systems in multidisciplinary contexts. In this talk, we will describe the research activities of our first cohort of undergraduates and the curricular enhancements in computational and data enabled science and engineering that have already been made. This project is supported by the NSF.

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MS74

Data-Enabled Science and Computational Analysis Research, Training, and Education for Students (descartes) Program at UC Merced

The Data-Enabled Science and Computational Analysis Research, Training, and Education for Students (DESCARTES) Program at UC Merced trains Applied Mathematical Sciences majors in the computational tools needed to study modeling and simulation of complex systems and analysis of large data sets. This program has three specific aims: (1) Provide exceptional undergraduate students unique research opportunities and state-of-the-art education and training in computational and data-enabled science; (2) Develop the Computational and Data-Enabled Science emphasis track within the Applied Mathematical Sciences Major; and (3) Provide high school math teachers from the region the opportunity to learn the tools and methods of computational and data-enabled science. In this talk, we will describe current developments within the DESCARTES program and discuss new initiatives that we have undertaken since the inception of the program.

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MS74

Computational and Data-Enabled Training in William & Mary

In this talk, I will talk about how EXTREEMS-QED is organized at W&M, how we recruit students, and how to run our summer research programs. I will also talk about how we develop Data-related courses.

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MS75

A Stochastic-Oriented NLP Relaxation for Integer Programming

We introduce a nonlinear, nonconvex relaxation of integer constraints in certain linear programs. The relaxation is motivated by the interpretation of relaxed integer variables as probability of units to be on in energy systems applications. The relaxation depends on a complexity parameter that controls its strength that is derived from a quantile interpretation of a stochastic formulation. We analyze the dependence of the solution on this complexity parameter and provide numerical examples to support our claims.

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MS75

Uncertainty Analysis of Wind Power Plant Dynamic Model

In transient stability studies, large wind power plants (WPP) are usually represented by reduced model consisting on one, or few, equivalent machines. However individual wind turbine generators (WTG), within a WPP, can produce diverse power outputs, because of terrain topography and/or wake effect. Under these conditions, the accuracy of the reduced WPP model has not been studied yet. In this paper, we present an uncertainty analysis to investigate the model accuracy of a WPP model under diverse power outputs of its individual WTGs. Wake effect is considered as the reason for diverse power outputs. The impact of wake effect in dynamic WPP model uncertainty is investigated. The importance of diverse WTG power output is evaluated in full and reduced models of a large 168-machine test WPP connected to the IEEE-39-bus system. The results show that diverse WTG output due to wake effect can affect the transient stability outcome analysis. The reduced WPP model misrepresents the dynamic response observed with the full WPP representation. Engineers should be aware of this difference when using reduced WPP models.

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MS75

Global Optimization of Large Optimal Power Flow Problems

We propose a global optimization algorithm based on branch and bound for the Optimal Power Flow (OPF) problem in power grids. The algorithm uses Semidefinite Programming (SDP) relaxations of the OPF to provide strong lower bounds on the optimal objective function value. The algorithm is able to guarantee global optimality to a small tolerance for several IEEE benchmark instances and modified instances, orders of magnitude faster than general purpose global optimization solvers. We also extend the algorithm to the smart grid problem, which is a multi period extension of the OPF to address integration of renewable energy sources and storage devices into the power grid. Results illustrate the effectiveness of storage in lowering costs and absorbing fluctuations due to intermittent power sources in the grid.

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MS75

Exploiting Large-Scale Natural Gas Storage to Mitigate Power Grid Uncertainty

We present a stochastic optimal control model to optimize gas network inventories in the face of system uncertainties. We demonstrate that gas network inventories can be used to mitigate volatility observed in power grid operations.

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MS76

Mathematical Models and Computational Software for Hazardous Earth-Surface Flows: from Tsunamis to Landslides

There is a large class of geophysical flows that can be categorized as hazardous, free-surface, gravity-driven inundating flows. These problems include tsunami propagation and inundation; overland flooding; hurricane-generated storm surges; and a range of granular-fluid flows including landslides, debris flows and lahars. These problems are often modeled with depth-averaged PDEs sharing common mathematical features and presenting similar computational challenges. I will describe these models and show simulations of tsunamis, floods and landslides using these methods.

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MS76

Dynamically and Kinematically Consistent Global Ocean State Estimation for Climate Research

The sparsity of observations for oceanographic (and cryospheric) research directed at climate requires the development and application of mathematical and computational tools, variously known as inverse methods, or state and parameter estimation, to infer poorly known or not directly measurable quantities, and to provide useful uncertainty estimates. Data assimilation commonly used in numerical weather prediction applies filtering methods that are optimal for forecasting. However, to the extent that the focus is on understanding the dynamics of the ocean's past evolution such methods have limitations; they do not preserve known conservation laws and evolution equations. Instead, climate reconstruction is best solved using smoother methods such that optimal use is made of the sparse observations while preserving known physical laws encapsulated in the model used for data interpolation. Two examples from global ocean state estimation and ice sheet modeling will be discussed.

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MS76

Computational Challenges in High-Resolution, Experimentally-Constrained Non-Newtonian Subduction Modeling

Results from high-resolution, massively parallel, three-dimensional numerical models of subduction zone deformation are presented. The models are observationally based, contain multiple plates, and use a non-Newtonian viscosity, making them among the highest fidelity convergent margin models to date. A scalable solver is used to solve the difficult variable viscosity stokes flow. Large viscosity gradients emerge due to the strain-rate dependent viscosity, allowing for local decoupling and complex circulation semi-independent from the larger scale mantle circulation.

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MS76

Promoting the Development and Application of Mathematics, Statistics and Computational Science in the Geosciences

I will begin by describing recent efforts of the Consortium for Mathematics in the Geosciences (CMG++) formed by members of the mathematical, statistical, computational and geoscience communities. The goal of the consortium is to accelerate traditional interactions between these groups of scientists. Then I will discuss a computational inverse method developed by myself and colleagues that was motivated by specific challenges in oceanographic data assimilation and geophysics.

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MS77

Imaging of Extended Reflectors in Two-Dimensional Waveguides

We consider the problem of imaging extended reflectors in waveguides using the response matrix of the scattered field obtained with an active array. We employ selective imaging techniques to focus onto the edges of a reflector which typically give raise to weaker echoes than those coming from its main body. A selective imaging functional based on Kirchhoff migration and the SVD of a weighted modal projection of the response matrix is proposed and analyzed.

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MS77

Imaging of Sparse Scatterers

Abstract not available at time of publication.

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MS77

Connecting the Dots: from Homogenization to Radiative Transport

Abstract not available at time of publication.

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MS77

Signal to Noise Ratio Analysis in Virtual Source Array Imaging

We consider imaging a reflector located on one side of a passive array where the propagation medium is homogeneous. The reflector is illuminated by remote impulsive sources situated on the other side of the passive array where the medium is complex and strongly scattering. We transform the passive array to an active virtual array by migrating the cross correlations of the field recorded on the passive array. We will present an analysis of the signal to noise ratio of the obtained image.

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MS78

Flagellar Kinematics of Algal Cells in Viscoelastic Fluids

The motility behavior of microorganisms can be significantly affected by the rheology of their fluidic environment. In this talk, we experimentally investigate the effects of fluid elasticity on both the flagella kinematics and swimming dynamics of the microscopic alga Chlamydomonas reinhardtii. We find that the flagellar beating frequency and wave speed are both enhanced by fluid elasticity. Interestingly, the swimming speeds during the alga power and recovery strokes are enhanced by fluid elasticity for De 1. Despite such enhancements, however, the alga net forward speed is hindered by fluid elasticity by as much as 30% compared to Newtonian fluids of similar shear viscosities. The motility enhancements could be explained by the mechanism of stress accumulation in the viscoelastic fluid.

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MS78

The Dynamics of Sperm Detachment from Epithelium in a Coupled Fluid-Biochemical Model of Hyperactivated Motility

A mechanical advantage of the spermatozoa hyperactivated waveform has been hypothesized to be the promotion of detachment from oviductal epithelium. Using a Stokes fluid model that incorporates forces due to dynamic elastic bonds between the flagellar head and a surface, we find that hyperactive waveforms do result in the frequent detaching and binding dynamics that are observed in recent lab experiments.

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MS78

The Phylogeny of Sperm Swimming Kinematics

Phylogenetic analyses have dominated the study of ecology and evolution. However, physical interactions between organisms and their environment are mediated by organism form and function, highlighting the importance of mechanics to understanding evolutionary trajectories. We combined high-speed video microscopy and singular value decomposition analysis to quantitatively compare the flagellar waveforms of sperm from eight diverse species. The emergence of dominant flagellar waveforms is suggestive of biological optimization, driven by environmental cues.

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MS78

Flagellar Bundling and Unbundling in E. Coli

Flagellar bundling and unbundling are important aspects of locomotion in bacteria such as Escherichia coli. To study the hydrodynamic behavior of helical flagella, we present a computational model that describes the motion of bacterial flagellar filament at the micrometer scale. Bundling occurs when all flagella are left-handed helices turning counterclockwise or when all flagella are right-handed helices turning clockwise. Helical flagella of the other combinations of handedness and rotation direction do not bundle.

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MS79

Unifying the Equations of Life: Time Scale Calculus and Evolutionary Dynamics

Evolutionary dynamics is concerned with the evolution of populations. In a general framework, each population has its own geometry, method of adaptation (incentive), and time-scale (discrete, continuous, and others). Using an information-theoretic measure of distance, a widely-applicable stability result will be given for all of these scenarios. A wealth of examples leading up to and beyond the main results is included. No prior knowledge of evolutionary dynamics, information theory, Riemannian geometry, or game theory is required.

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MS79

Flight Stability of Mosquitoes using a Reduced Model

We employ a reduced model that represents a mosquito as a rigid body with two rigid wings to explore mosquito stability. Wing motions derived from analysis of high speed movies are used as inputs to a dynamical model of the mosquito body. We study uniform flight where flight trajectories are periodic orbits in a suitable translating reference frame. We analyze the stability of body motions in this frame by computing a linearized return map of the periodic orbit along with its eigenvalues and singular values. Long time stability corresponds to eigenvalues all smaller than one in magnitude and depends upon model parameters. For our mosquito geometry, we find that hovering flight is unstable but locate parameter ranges in which forward flight is stable. We also investigate the effect of varying the location of the joint between wings and body on stability of hovering flight. All cases are close to marginal stability.

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MS79

On a Non-Linear Investigation of An Electrospinning Model under Combined Space and Time Evolving Instabilities

We study the nonlinear problem of axisymmetric electrically driven jets with applications to the electrospinning process. We consider classical stability point of view in the early stage and then weakly nonlinear wave theory of certain dyad resonance modes that later involve the use of Newton's Method to solve a dispersion relation. Finally we present the Method of Lines (MOL) to solve a system of PDEs that governs the combined time and space evolving amplitude instability functions.

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MS79

Analyzing Coherent Structure in Signals and Fluid Flows

We consider a dynamical systems based method for measuring the complexity of particle trajectories in fluid flows. This complexity is measured in terms of ergodicity which relates to how a trajectory samples a space and how it samples provides insight about the structure in the phenomena or region of interest. We discuss how this insight is used to visualize the 2D and 3D Lagrangian coherent structures in ocean flows and how this information can in turn be used to better understand the transport in the flow - e.g., transport barriers and transport facilitators. As time permits, other related diagnostics will also be presented.

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MS80

Asymptotically Compatible Schemes for Robust Discretization of Nonlocal Models

We present an abstract framework of asymptotically compatiable (AC) schemes for robust discretizations of a family of parametrized problems. The AC schemes provide convergent approximations to problems associated with fixed parameter values as well as their limiting values. This framework is then applied to study approximations of nonlocal models such as peridynamic models of nonlocal elasticity parametrzed by the horizon parameter and their local PDE limits (Navier equations) when the horizon parameter approaches zero. In particular, by combining with the theory of nonlocal calculus of variations, a precise characterization of AC schemes can be obtained for popular conforming finite element discretizations.

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MS80

Analysis and Approximation of Finite-Range Jump Processes

The classical Brownian motion model for diffusion is not well-suited for applications with discontinuous sample paths. For instance, the mean square displacement of a diffusing particle undergoing a jump process often grows faster than that for the case of Brownian motion, or grows at the same rate but is of finite variation or finite activity. Such jump processes are viable models for anomalous super-diffusion or nonstandard normal diffusion. In particular, such jump diffusions are expedient models when the process sample-path is discontinuous because nearly instantaneous price volatility, species migration or heat conduction is suggested by the length and time scales over which the data is collected. My presentation is on recent work for the associated deterministic equation on bounded domains where the jump process is of finite-range, i.e, the jump-rate is positive over a region of compact support. We refer to the associated deterministic equation as a volume-constrained nonlocal diffusion equation. The volume constraint is the nonlocal analogue of a boundary condition necessary to demonstrate that the nonlocal diffusion equation is well-posed and be consistent with the jump process.

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MS80

Modeling Anomalous Diffusion Using the Fractional Bloch-Torrey Equation

Contrast in magnetic resonance imaging (MRI) can be manipulated to display the apparent diffusion coefficient for water. In complex, heterogeneous materials, such as biological tissue, diffusion is anisotropic and often non-Gaussian. Such anomalous diffusion can be succinctly described via the fractional order Bloch-Torrey equation - a FPDE that captures both deterministic and stochastic processes. Using this model, MRI can display spatial maps of tissue properties in terms of sub- and super-diffusion.

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MS80

Fractional PDEs: Numerical Methods and Mathematical Analysis

We present a faithful and efficient numerical methods for time-dependent space-fractional PDEs in three space dimensions, without resorting to any lossy compression, but rather by exploring the structure of the coefficient matrices. The method reduces computational cost from $O(N^3)$ to $O(N \log^2 N)$ per time step and memory requirement from $O(N^2)$ to $O(N)$. We also address some mathematical issues that are characteristic for fractional PDEs and report our recent progress in this direction.

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MS81

BANDITS: A Matlab Package of Band Krylov Subspace Iterations

Band Krylov subspace iterations are extensions of Krylov subspace methods such as the Arnoldi process and the Lanczos algorithm, which can handle only single starting vectors, to the case of multiple starting vectors. Band methods have a number of advantages over the more traditional block Krylov subspace methods. We describe the Matlab package BANDITS that provides implementations of band versions of the Arnoldi process, the general Lanczos method, and the symmetric and Hermitian Lanczos algorithms.

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MS81

Newton-Krylov Method for Problems with Embed-

ded Monte Carlo Simulations

We analyze the behavior of inexact Newton methods for problems where the nonlinear residual, Jacobian, and Jacobian-vector products are the outputs of Monte Carlo simulations. We propose algorithms which account for the randomness in the iteration, develop theory for the behavior of these algorithms, and illustrate the results with an example from neutronics.

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MS81

The Lanczos Algorithm and Extensions for Quaternionic Matrices

Let $\mathcal{A}$ be an associative algebra containing one and $\mathbf{A}$ a square matrix with entries from $\mathcal{A}$. Let there be a vector $\mathbf{x} \neq 0$ with entries from $\mathcal{A}$ and $\lambda \in \mathcal{A}$ such that

$$\mathbf{A}\mathbf{x} = \mathbf{x}\lambda, \tag{1}$$

where the multiplication on the right is carried out componentwise. Then, λ will be called an *eigenvalue of* $\mathbf{A}$ associated with an *eigenvector* $\mathbf{x}$ of $\mathbf{A}$. If we multiply (1) from the right by an invertible element $h \in \mathcal{A}$ we obtain

$$\mathbf{A}[\mathbf{x}h] = \mathbf{x}\lambda h = [\mathbf{x}h]\,[h^{-1}\lambda h], \tag{2}$$

which shows that the set of eigenvalues of quaternionic matrices can always be reduced to complex numbers. This is not necessarily so in other algebras. The Lanczos algorithm produces a series of tridiagonal $j \times j$ matrices $\mathbf{T}_j$, $j = 1, 2, \ldots$ from a symmetric matrix $\mathbf{A}$, and the eigenvalues of $\mathbf{T}_j$ (called *Ritz values*) approximate the eigenvalues of $\mathbf{A}$ (usually very quickly). We report on the results for quaternionic matrices and on extensions to other noncommutative algebras. Algebraic operations with quaternions are in general more effective than the corresponding operations with their matrix counterpart. This research was supported by the DFG, GZ OP 33/19-1

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MS81

Hierarchical Krylov and Nested Krylov Methods Using PETSc for Extreme-Scale Computing

We develop hierarchical Krylov methods and nested Krylov methods to overcome the scaling difficulties for extreme-scale computing. We demonstrate the impact at high core counts on the PFLOTRAN subsurface flow application. Because these algorithms can be activated at runtime via the PETSc library, application codes that employ PETSc can easily experiment with such techniques. The principles of hierarchal Krylov methods and nested Krylov methods can be applied to complementary advances in synchronization and communication-avoiding Krylov methods, thereby offering potentially multiplicative benefits of combined approaches.

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MS82

Information Theoretic Projection of Cytoskeleton Dynamics onto Surrogate Cellular Motility Models

Lattice Boltzmann and lattice Fokker-Planck methods can readily handle the geometric and physical complexity of the reactions underlying cytoskeleton formation and dynamics from actin polymerization and myosin motor motion. The computational cost, even for such simplified discretizations of the flow velocity and cytoskeleton configuration, is still prohibitive for study of cellular motion over many cell diameters. This talk presents a non-linear projection approach to the construction of surrogate models of cellular motility, as extracted from lattice computations. A mesoscale state is represented by a set of parameters from a family of probability density functions. The non-linear projection is induced by geodesic transport in the non-Euclidean geometry of the space of probability functions, guided by information theoretic functionals that quantify the fidelity of a reduced model. Several interesting links between microscopic parameters governing cytoskeleton formation and overall cell motion are brought out by this approach.

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MS82

Hybrid Models and Interfaces

In various applications the traditional mathematical models based on PDEs, with their empirically determined coefficients, and associated traditional numerical approximations, are not sufficient to describe all the relevant dynamics and complexity. In the talk we describe our progress on hybrid computational models which combine traditional numerical PDEs with other computational methods from, e.g., statistical mechanics, and more broadly computational physics. We focus on a model which accounts for complicated physics occuring at a fixed interface in semiconductors, which involves a Density Function Theory model at microscale and a Domain Decomposition approach involving a traditional drift-diffusion equation at macroscale.

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MS82

Lagrangian Particle Methods for Multiphase Flows

Here we present a novel formulation of the so-called multiphase Pairwise Force Smoothed Particle Hydrodynamics Method originally proposed by Tartakovsky and Meakin.

We derive a relationship between parameters in the pairwise forces and the surface tension and static contact angle, validate the model and demonstrate its applicability for studying complex processes such as multiphase flow in porous media with variable wettability.

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MS82

Modeling Nanoscale Fluid-Solid Interfaces

Structure and dynamics of soft matter are governed by molecular interactions and hydrodynamic fluctuations. As the molecular and hydrodynamic aspects are coupled, computer simulations of soft matter must confront this multiscale challenge. I will present a new scale-consistent simulation framework that combines molecular dynamics (MD) and fluctuating hydrodynamics (FHD) to enable multiscale modeling of complex systems. This method allows resolution of solute-solvent interfaces and realization of excluded volumes of particles in the presence of hydrodynamic coupling. Simulation results show that the hybrid FHD/MD method can reproduce the solvation free energies and scaling laws of particles dynamics for hydrophobes of difference sizes. Simulations of self-assembly of hydrophobic particles will also be presented.

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MS83

Persistence Modules and their Applications to Material Sciences

In this talk, we present several applications of persistence modules to material sciences such as proteins and glasses. The types of persistence modules are given by representations on A_n-quiver (i.e., standard persistent homology) and on commutative triple ladder quivers. Furthermore, we give a generalized notion of persistence diagrams which is defined as a graph on Auslander-Reiten quivers. Some of the computational results applied to proteins and glasses are also shown.

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MS83

Analyzing the Dynamics of Pattern Formation in the Space of Persistence Diagrams

Persistence diagrams are a relatively new topological tool for describing and quantifying complicated patterns in a simple but meaningful way. We will demonstrate this technique on patterns appearing inRayleigh-Benard convection. This procedure allows us to transform experimental or numerical data from experiment or simulation into a point cloud in the space of persistence diagrams. There are a variety of metrics that can be imposed on the space of persistence diagrams. By choosing different metrics one can interrogate the pattern locally or globally, which provides deeper insight into the dynamics of the process of pattern formation. Because the quantification is being done in the space of persistence diagrams this technique allows us to compare directly numerical simulations with experimental data.

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MS83

Reconstructing Manifolds and Functions from Point Samples

We will survey some fantastic work of Niyogi, Smale and Weinberger which provides explicit bounds on the number of sample points required to reconstruct an underlying manifold up to homotopy type with high confidence. Next, we imagine the situation where an unknown function between two such manifolds must be inferred from point samples along with the ability to evaluate the function at the domain-samples. Not only can such functions be reconstructed up to homotopy from finite point samples with high confidence, but also that the entire process of reconstruction is robust to certain models of sampling and evaluation noise.

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MS83

Word Representations of Structurally Stable Hamiltonian Flows in Multiply Connected Domains and its Applications

We consider Hamiltonian vector fields with a dipole singularity that satisfy the slip boundary condition in two-dimensional multiply connected domains. One example of such a Hamiltonian vector field is the incompressible and inviscid flow in an exterior multiply connected domain in the presence of a uniform flow whose Hamiltonian is called the stream function. They are regarded as mathematical models of biofluids, rivers and coastal flows. Here, we are interested in structurally stable Hamiltonian vector fields and their topological structures of contour lines of the Hamiltonian, i.e. streamline patterns. We develop an encoding procedure to assign a unique sequence of words to every streamline pattern. Owing to this word representation, we not only determine all possible streamline patterns in a combinatorial manner, but also describe the complex evolution of fluid flows as a change of words. Moreover, we can determine possible transitions between two different structurally stable streamline patterns. In the present talk, we introduce the theory of word representations for structurally stable Hamiltonian vector fields and demonstrate how it is applicable to fluid flow problems with vortex structures.

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MS85

High-Order Algorithms for Compressible Reacting Flow with Complex Chemistry

We describe a numerical algorithm for integrating the multicomponent, reacting, compressible Navier-Stokes equations, targeted for direct numerical simulation of combustion phenomena. The algorithm addresses two shortcomings of previous methods. First, it incorporates an eighth-order narrow stencil approximation of diffusive terms that reduces the communication compared to existing methods and removes the need to use a filtering algorithm to remove Nyquist frequency oscillations that are not damped with traditional approaches. The methodology also incorporates a multirate temporal integration strategy that provides an efficient mechanism for treating chemical mechanisms that are stiff relative to fluid dynamical time scales. The overall methodology is eighth order in space with option for fourth order to eighth order in time. The implementation uses a hybrid programming model designed for effective utilization of many-core architectures. We present numerical results demonstrating the convergence properties of the algorithm with realistic chemical kinetics and illustrating its performance characteristics. We also present a validation example showing that the algorithm matches detailed results obtained with an established low Mach number solver.

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MS85

High-Order Numerical Methods for Fractional PDEs in Water Wave Propagation

We consider numerical solutions for a fractional PDE arising as a nonreflecting boundary condition in water wave propagation. The fractional derivative is expressed as divergence of a singular integrable convolution. The equation is viewed as a linear conservation law with a nonlocal singular flux. A semi-discrete finite volume scheme uses local polynomial approximation of order p from solution cell averages, followed by exact integration of the singular flux, and yields a surprising convergence rate of $p + 3/2$. Time integration uses Runge-Kutta methods of matching order. We discuss stability and convergence, and show numerical results for uniform and nonuniform grids.

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MS85

Semi-Lagrangian Discontinuous Galerkin Schemes for the 2+2 Vlasov-Poisson System on Unstructured Meshes

The Vlasov-Poisson system is a set of equations that describe collisionless plasma far from thermodynamic equilibrium. Numerical difficulties in solving the Vlasov-Poisson system include the high-dimensionality and severe time step restrictions attributed to moderate to large velocities in the system. Explicit Eulerian methods require excessively small time steps, and implicit Eulerian methods have matrices with large condition numbers. Particle in Cell methods together with their Lagrangian and semi-Lagrangian counterparts relax this time step restriction by solving for the characteristics in the system. We propose a high-order operator split DG method for solving the Vlasov-Poisson system. Our hybrid method incorporates large time steps using semi-Lagrangian methods, and complicated geometries in configuration space with unstructured grids. We present 2D-2V results including the formation of a plasma sheath in the proximity of a cylindrical Langmuir probe, as well as the simulation of a single-species charged particle beam in an accelerator.

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MS85

Evaluation of Discrete and Continuous Adjoint Approaches for Sensitivity Analysis and Error Estimations for Numerical Approximations of Hyperbolic Pdes with Shocks

The literature on adjoint methods for shock-hydrodynamic applications is actually rather sparse and recent. Early investigations with continuous adjoint problems required accurate knowledge of the discontinuities. Recent work has shown that this issue may be mitigated by considering an alternative dual problem based on the concept of limiting viscocity. We compare and evaluate this approach using either a discontinuous Galerkin approximation or a continuous Galerkin approximation with flux-corrected transport for shock-hydrodynamic applications.

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MS86

Energetic Variational Approaches in Ion Transport

Almost all biological activities involve transport of charged ions in specific biological environments. In this talk, I will discuss a unified energetic variational approach developed specifically for these multiscale-multiphysics problems. I will discuss the relevant classical theories and relevant physical approaches and methods. I will focus on the mathematics, in particular the analytical issues arising from these studies.

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MS86

From Micropolar Navier Stokes to Ferrofluids, Analysis and Numerics

The Micropolar Navier-Stokes Equations (MNSE), is a system of nonlinear parabolic partial differential equations coupling linear velocity, pressure and angular velocity, i.e.: material particles have both translational and rotational degrees of freedom. The MNSE is a central component of the Rosensweig model for ferrofluids, describing the linear velocity, angular velocity, and magnetization inside the ferrofluids, while subject to distributed magnetic forces and torques. We present the basic PDE results for the MNSE (energy estimates and existence theorems), together with a first order semi-implicit fully-discrete scheme which decouples the computation of the linear and angular velocities. Similarly, for the Rosensweig model we present the basic PDE results, together with an fully-discrete scheme combining Continuous Galerkin and Discontinuous Galerkin techniques in order to guarantee discrete energy stability. Finally, we demonstrate the capabilities of the Rosensweig model and its numerical implementation with some numerical simulations in the context of ferrofluid pumping by means of external magnetic fields.

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MS86

Optimal Energy Norm Error Estimates for a Mixed FEM for a Cahn-Hilliard-Stokes System

In this I talk describe a mixed finite element method for a modified Cahn-Hilliard equation coupled with a non-steady Darcy-Stokes flow that models phase separation and coupled fluid flow in immiscible binary fluids and diblock copolymer melts. The time discretization is based on a convex splitting of the energy of the equation. I show that the scheme is unconditionally energy stable and unconditionally uniquely solvable and that the discrete phase variable is bounded in $L^\infty\left(0,T;L^\infty\right)$ and the discrete chemical potential is bounded in $L^\infty\left(0,T;L^2\right)$, for any time and space step sizes, in two and three dimensions, and for any finite final time T. With this in hand I show that these variables converge with optimal rates in the appropriate energy norms in both two and three dimensions. I will describe how this analysis can be extended to two-phase diffuse interface models with large density mismatch. This is joint work with Amanda Diegel and Xiaobing Feng.

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MS87

Generalized Multiscale Finite Element Methods for Wave Propagation in Heterogeneous Media

Numerical modeling of wave propagation in heterogeneous media is important in many applications. Due to the complex nature, direct numerical simulations on the fine grid are prohibitively expensive. It is therefore important to develop efficient and accurate methods that allow the use of coarse grids. In this talk, we present a multiscale finite element method for wave propagation on a coarse grid. To construct multiscale basis functions, we start with two snapshot spaces in each coarse-grid block where one represents the degrees of freedom on the boundary and the other represents the degrees of freedom in the interior. We use local spectral problems to identify important modes in each snapshot space. To our best knowledge, this is the first time where multiple snapshot spaces and multiple spectral problems are used and necessary for efficient computations. These multiscale basis functions are coupled via the symmetric IPDG method which provides a block diagonal mass matrix, and, consequently, results in fast computations in an explicit time discretization. Our methods' stability and spectral convergence are rigorously analyzed. Numerical examples are presented to show our methods' performance. The research is supported by Hong Kong

RGC General Research Fund (Project number: 400411).

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MS87

Maximal Laplace-Beltrami Eigenvalues on Compact Riemannian Surfaces

Let (M, g) be a connected, compact Riemannian surface and denote by $\lambda_k(M, g)$ the k-th eigenvalue of the Laplace-Beltrami eigenproblem. We consider the mapping $(M, g) \mapsto \lambda_k(M, g)$. We propose computational methods for solving the eigenvalue optimization problem of maximizing $\lambda_k(M, g)$ as g varies within a conformal class $[g_0]$ of fixed volume and for the problem where M is additionally allowed to vary over surfaces with fixed genus. Several properties are also studied computationally, including uniqueness, symmetry, and eigenvalue multiplicity.

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MS87

A Level Set-Adjoint State Method for the Joint Transmission-Reflection First Arrival Traveltime Tomography

We propose an efficient partial differential equation (PDE) based approach to the joint transmission-reflection traveltime tomography using first arrivals. In particular, we consider only the first arrivals from the transmission and reflection measurements at a series of receiver-source pairs. Unlike typical reflection tomography where the location of the reflector is assumed to be known by some migration techniques, we propose an efficient numerical approach based on the adjoint state method and the PDE based local level set method to invert both the piecewise smooth velocity within the computational domain and the location of a codimension-one reflector. Since we are using only first arrivals for tomography, we might not be able to obtain a perfect illumination of the reflector because the relevant information might be carried by the later arrivals. In this work, we propose an easily computed quantity which can quantify the reliability of our reconstruction. Numerical examples in both two- and three-dimensions will be given to demonstrate the efficiency of the proposed approach. The work is supported in part by the Hong Kong RGC under Grant GRF603011.

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MS87

Fast Matrix-free Direct Solution and Selected Inversion for Seismic Imaging Problems

Fast direct solvers have been shown very useful for modeling large inverse problems. In this talk, we show our recent development of matrix-free direct solvers for large dense or spare matrices based on rank structures and randomized sampling. Unlike existing direct or iterative methods, these new solvers can quickly provide direct solutions with controllable accuracies, using only a small number of matrix-vector multiplications. This is especially attractive for problems which are ill-conditioned, where it is too expensive to form the matrix, or where there are too many right-hand sides. The solvers are also useful for problems with varying parameters (e.g., frequency). We then discuss the application of the methods to the extraction of selected entries of the inverse of large sparse matrices. For discretized Helmholtz equations, we can quickly compute the diagonal blocks or any off-diagonal entries of the inverse. Such information is useful for the preconditioning of the problem. These methods can significantly improve the efficiency of the solution/inversion of the Hessian matrix in Gauss-Newton iterations for FWI.

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MS88

The Scholarly Work of Reliable and Well-Designed Mathematical Software

Well-designed mathematical software has long been considered a cornerstone of scholarly contributions in computational science. Forsythe, founder of Computer Science at Stanford and regarded by Knuth as the "Martin Luther of

the Computer Reformation," is credited with inaugurating the refereeing and editing of algorithms not just for their theoretical content, but also for design, robustness, and usability. His vision extends to the current day, and this talk presents a modern perspective of academic software. The speaker's academic software constitutes much of x=A\b in MATLAB when A is sparse, and is widely used in many other academic, government, and commercial applications, because of its performance and its reliability.

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MS88

A Deterministic Guaranteed Automatic Algorithm for Univariate Function Approximation

Function recovery is a fundamental computational problem. It is desirable to have automatic algorithms for solving such problems, i.e., the algorithms decide adaptively how many and which pieces of function data are needed and then use those data to construct an approximate function. The error of this approximation should be guaranteed not to exceed the prescribed tolerance. We provide a deterministic guaranteed automatic algorithm for univariate function approximation on a given finite interval and prove its reliability.

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MS88

A Survey of Issues in Reliable Computational Science

Continuing developments in computing software and hardware allow us to solve more complex problems than ever before. However, there remains the nagging question of how we can be sure that the answers are correct. This talk surveys the efforts that have been made to ensure that computational science is reliable and the work that still needs to be done.

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MS88

Generation of Appropriate Publication Citations by Numerical Software Libraries

Properly citing academic publications that describe software libraries and algorithms is the way that open source scientific library users "pay" to use the free software. With large multifaceted libraries and applications that use several such libraries, even the conscientious user may end up citing publications in error or missing relevant publications. Based on a feature recently added to the PETSc numerical software libraries, we suggest an alternative model where the library itself generates the bibtex items based on exactly what algorithms and portions of the code are used in the application.

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MS89

The Inverse Fast Multipole Method

We present a fast direct solver for dense linear systems arising out of wide range of applications, integral equations, multivariate statistics, radial basis interpolation, etc., to name a few. *The highlight of this new fast direct solver is that the solver scales linearly in the number of unknowns in all dimensions.* The solver, termed as the Inverse Fast Multipole Method, works on the same data-structure as the Fast Multipole Method. More generally, the solver extends to the class of hierarchical matrices, denoted as $\mathcal{H}^2$ matrices with strong admissibility criteria, i.e., *only the interaction between particles corresponding to well-separated clusters is represented as a low-rank matrix*, and thereby the algorithm departs from the existing (HSS/ HODLR) approaches. We also present numerical benchmarks in 1D and 2D validating the linear scaling of the algorithm.

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MS89

Hierarchical Interpolative Factorization

We present some recent results on the efficient factorization of matrices associated with non-oscillatory integral operators in 2D and 3D. In contrast to the 1D case, such matrices exhibit considerable rank growth in their off-diagonal blocks when compressed using standard hierarchical schemes. We combat this with explicit dimensional reductions via geometric reclustering and additional compression. The resulting ranks are much better behaved, yielding essentially linear costs to construct, apply, and invert the factorization. Our method is fully adaptive and can handle both boundary and volume problems.

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MS89

Randomized Methods for Accelerating Structured Matrix Computations

Randomized methods have over the last several years proven to be powerful tools for computing low-rank approximations to matrices whose singular values exhibit appropriate decay. In this talk, we describe how such techniques can be extended to certain "rank-structured" matrices, for which only certain off-diagonal blocks (not the matrix itself) admit accurate low-rank approximations. Matrices of this type often arise in the construction of O(N) direct solvers for elliptic PDEs.

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MS89

Parallel Structured Direct Solvers for Nonsymmetric and Indefinite Sparse Matrices

Fast structured direct solvers have been extensively studied for matrices with a low-rank property. Most existing work concentrates on symmetric and/or positive definite problems. Here, we exploit this structure in the direct solution of nonsymmetric and indefinite matrices. Graph ordering and pivoting are performed. The pivoting strategy is designed in a way so as to preserve both the sparsity and the rank structure. A structured multifrontal LU factorization is then performed. To implement the method in parallel, we use static mapping to preallocate tasks to processes. Under a certain switching level in the tree, factorizations are done locally in each process. Beyond the switching level, processes of child nodes form a process grid on parent nodes where structured operations are performed among the processes. In such a way, both idling and communications are reduced. All the frontal and update matrices are structured and their factorizations are done in parallel. In the numerical experiments, we show the applications of this method to seismic imaging and more general problems. This is joint work with Jianlin Xia.

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MS91

A Fully Implicit Approach for the Solution of Temporal Multiscale Problems with Application to Power Grid

In this talk, we present a fully implicit approach for temporal multiscale problems and discuss a power grid application that involves two time-scales. At each step of the slow time-scale, our approach involves solving equations for one step of the slow time-scale along with several coupled-in-time equations for the fast time-scale. We will discuss the formulation, preconditioning techniques, and parallel implementation of our approach.

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MS91

Gridpack Toolkit for Developing Power Grid Simulations on High Performance Computing Platforms

This presentation describes the GridPACK framework, which is designed to help power grid engineers develop modeling software capable of running on todays high performance computers. The framework contains modules for managing power grid networks, distributed matrices and vectors, parallel linear and non-linear solvers, and mapping functionality to create matrices and vectors based on properties of the network. Examples of applications built with GridPACK will be presented and performance results will be discussed.

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MS91

Power Grid Simulation: Needs, State of the Art, Challenges

The complexity of Power Grid is increasing, due to the massive integration of intermittent generation far away from load centers or dispersed in the distribution grids. The Power Grid is operated nearest to its limits; more and more closed loop controls are installed in the system. There is an urgent need to base decisions on a more accurate description of the system including its dynamic behavior. The Power Grid simulation must now include time domain simulation and not only static Power Flow. Most of the Power Grid Simulation tools use fixed time step methods and hard coded modeling of the components even if only variable time step implicit method can offer a certain level of confidence for the accuracy of the results in particular at the design stage when the dynamic behavior could be far away from a realistic and expected behavior. A tough requirement is that physical unstable Power Grid must be simulated as unstable. The "over damping" intrinsically induces by numerical methods which guarantees the damping of numerical errors, must be minimized as much as possible.

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MS91

Experiences with Time Integration Algorithms in

a Time Domain Simulation Code

Commercial power grid simulators often employ a standard Trapezoid time integration scheme along with constant time steps for their time evolution. In this talk we will discuss our experiences in incorporating a variable step integrator within a commercial time domain simulation code. The method used includes a second order predictor and a time step selector based on controlling local truncation error. Preliminary results show potential for significant speedup in simulation runs.

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MS92

Mathematics Research: Support, Stakeholders, Accountability

The papers we publish and read are crucial to us as researchers. However, there are many other stakeholders of mathematical publishing as well: our employers, organizations like SIAM, corporate publishers, funding agencies, and society, which ultimately pays for and benefits from the research. The diverse requirements of stakeholders, together with rapidly advancing technology and economic and social factors have created turmoil and sometimes conflict in publishing, placing us in a time of both peril and opportunity.

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MS92

Mathematics and Science Policy: Some Perspectives from SIAM's President

Mathematical sciences are a common denominator behind key scientific and technological advance, from robotics and genetics to Big Data, reminding us all of the vital importance of a well-trained STEM community to the future. Accordingly, SIAM plays a pivotal role promoting the visibility of mathematics in the halls of government, contributing to science policy discussions, all the while advocating for much-needed research dollars and resources to improve STEM education.

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MS92

Building Support, Building Budgets for the Mathematical Sciences

I will provide some perspectives on how federal science budget requests are built; what kinds of arguments seem to be effective for increasing requests; and what actions the mathematical sciences community can take to justify and support such requests.

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MS92

SIAM's Initiatives and Activities in STEM Education

In this talk SIAM's initiatives in STEM education, and their relations to science policy will be discussed. Important aspects of this are the Modeling across the Curriculum, MaC, initiative. The two MaC workshops (August 2012 and January 2014) and their outcomes will be presented. Other important recent activities include the INGenIOuS project which exemplified the way various mathematical sciences professional societies can work together to enhance understanding of the issues and affect policy.

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MS93

Crop Rotation Modeling and Optimization for Sustainable Water Use

We use a simulation-based optimization framework to guide planting decisions with a constraint to account for sustainable water usage. The motivation is the berry farming region of the Pajaro Valley, CA, which is overdrawing from the aquifer, resulting in seawater intrusion. MODFLOW-FMP is treated as a black-box with optimization tools from DAKOTA. We compare modeling formulations and optimization algorithms to understand trade-offs and identify challenges.

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MS93

Estimating Uncertainty in Annual Energy Production

A primary quantity in the evaluation of a proposed solar power plant is the annual energy production (AEP). Uncertainty in the AEP is often quantified by estimating the 50th and 10th percentiles by means of a model. The ratio between these quantiles significantly affects the financial risk associated with the proposed power plant, and thus, uncertainty in AEP significantly impacts a proposals success. We outline a method for estimating uncertainty in annual energy accounting for the three primary contributions to this uncertainty: inter-annual variability in the weather; uncertainty in measurements of irradiance; and modeling error in the translation from irradiance to power. We describe how this can be used to improve AEP uncertainty estimates in Arizona and Georgia.

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MS93

Analysis of a Managed Aquifer Recharge System

Over the last few decades, groundwater resources have been depleted at a faster rate than the underlying aquifers have been replenished. This imbalance has led water management agencies to consider managed aquifer recharge networks, where infiltration basins are used to replenish the aquifers using previously uncaptured storm water runoff. In this work, we utilize optimization to evaluate the costs associated with constructing such a network while simultaneously meeting demands placed on the aquifer. We present results for a realistic subwatershed in the Pajaro Valley region of California. We utilize existing computational tools to determine limits for the constraint equations, to compute subwatershed drainage areas, and to compute the corresponding storm water runoff over a predetermined time period consisting of several rain events. We present results that may be used to suggest best practices with regards to regional recharge basin design.

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MS93

Modeling Impacts of Water Level Control Procedures on Water Quality of the St Lawrence River

The St Lawrence River is the 13th largest river on the earth and the greatest single fluvial point source of freshwater to the North Atlantic. This river is faced with important ecosystem management issues related to the interdependence of environmental issues, e.g., the effect of climate change on invasive species, nutrient processing, and water budgets. Our work focus on development of integrated modeling techniques to explore the interplay of nutrient loading and population dynamics as modulated by the water control procedures implement to maintain nearly neutral levels. Our work seeks to understand the impact of more natural level excursions in the river that might be considered as a way to maintain the nearshore ecosystem.

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MS94

Discovery of Principles of Nature from Matrix and Tensor Modeling of Large-Scale Molecular Biological Data

We will describe the use of matrix and tensor decompositions in comparing and integrating different types of large-scale molecular biological data, from different studies of cell division and cancer and from different organisms, to computationally predict previously unknown physical, cellular and evolutionary mechanisms that govern the activity of DNA and RNA. We will present novel generalizations of the singular value decomposition as well as experimental verification and validation of some of the computational predictions.

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MS94

Deconvolution of the Mammalian Cell Cycle Metabolome

We have completed a comprehensive mass spectrometry analysis quantifying hundreds of small molecule metabolites throughout the phases of the mammalian cell cycle. Using singular value decomposition of the matrix of metabolite abundance from a synchronized culture of HeLa cells, we have produced a map of metabolic changes by phase of cycle, allowing the characterization of the coordinated metabolic changes occurring in the proliferating human tumor cell.

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MS94

Tensor Completion Methods in Seismology: Reconstruction, Denoising and Un-Mixing Seismic Sources

Seismic data can be stored in 5D tensors that depend on time (or frequency), x-y position of receivers, and x-y position of sources. This talk will discuss the development of algorithms, inspired by tensor algebra and recent work on nuclear norm minimization, to de-noise and reconstruct large 5D volumes of seismic data. I will also discuss the application of tensor algebra techniques to the problem of seismic source separation. The latter arises when seismic data are acquired with sources that are triggered almost simultaneously in order to save acquisition time.

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MS94

Coherent Pattern Detection in Tensor Data

In real-world applications, multidimensional data may contain coherent patterns and we need to perform clustering simultaneously along all dimensions of the data to detect these patterns. In this talk, we will discuss how column-pair based strategies we have developed for biclustering 2D data can be extended to higher dimensions. We can use tensor decomposition algorithms to convert a complicated coherent pattern detection problem in a high dimensional data space to simpler 2D data analysis problems.

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MS95

A Spectral Analysis for Regularization and Image Processing Applications

Regularization incorporates prior information into mathematical models to favor desired solutions. When computing piecewise polynomial solutions whose derivatives of certain order are sparse, a common regularizer is the L1-norm of the derivatives. Our interest evolved from the fact that approximations to the desired solution are often more accurate, up to orders of magnitude, than approximations to the derivatives. We explain such a phenomenon by a spectral analysis of discrete derivatives and propose alternative regularizers.

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MS95

Exploiting Nonlinear Structure for Nonconvex Optimization

Many important design and operational planning problems give rise to nonconvex optimization problems. We review the reformulation-linearization technique (RLT) for solving certain polynomial optimization problems to global optimality. We show how to exploit nonlinear structure in RLT, such as partial separability, and present numerical results that show that the resulting relaxation can be solved orders of magnitude faster.

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MS95

Topology Control for Load Shed Recovery

We introduce the dc optimal load shed recovery with transmission switching model (DCOLSR-TS), which seeks to reduce potential post-contingency load shedding by modifying the system topology. Since solving DCOLSR-TS is computationally difficult, we develop a heuristic (MIP-H), which improves the system topology while specifying the sequence of switching operations. We argue the use of a parallelized version of MIP-H for on-line load shed recovery and recurring contingency-response analysis.

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MS95

A Coxian-Phased Approximation for Border Crossing Service Times of Commercial Trucks

Since 2011, yearly combined trade exceeds $1 trillion within North American nations, with 80% transported by commercial trucks. Previous analytical models assume Markovian distributions for service time. Yet, field data lacks fit, and security procedures such as canine detection create dependencies. This research presents an analytical model of the border crossing process with an implementation of Mixture of Generalized Erlang (MGE) distributions, also known as Coxian k-phased distributions, as an improved inspection service time approximation.

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MS96

A Fast Finite-Volume Eulerian-Lagrangian Localized Adjoint Method for Space-Fractional Advection-Diffusion Equations

Fractional advection-diffusion PDEs provide an adequate and accurate description of subsurface flow and transport processes in porous media that exhibit anomalous diffusion, which can not be modeled properly by second-order advection-diffusion equations. However, fractional advection-diffusion PDEs raise mathematical and numerical difficulties that have not been encountered in the context of second-order advection-diffusion PDEs. In this talk we present a faithful and fast finite-volume Eulerian-Lagrangian localized adjoint method for space-fractional advection-diffusion equations, without resorting to any lossy compression, but rather by exploring the structure of the coefficient matrices. These methods have computational cost of O(N log2 N) per time step and memory of O(N), while retaining the same accuracy and approximation property of the underlying numerical methods.

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MS96

Variational Formulation of Problems Involving Fractional Order Differential Operators

In this talk, we consider boundary value problems involving either Caputo or Riemann-Liouville fractional derivatives of order $\alpha \in (1, 2)$ on the unit interval $(0, 1)$. The variational problem for the Riemann-Liouville case is coercive on the space $H_0^{\alpha/2}(0, 1)$ but the solutions are less regular, whereas that for the Caputo case involves different test and trial spaces. We establish the regularity pickup of the solutions of the variational problem, which enables one to establish convergence rates of the finite element approximations. The analytical theory is then applied to the Sturm-Liouville problem involving a fractional derivative in the leading term. Finally, extensive numerical results are presented to illustrate the error estimates.

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MS96

High Order Scheme for Caputo Derivative and Its Application to Caputo Type Advection-Dispersion Equation

In this paper, we derive a high order numerical scheme for $\alpha(\in (0, 1))$-th order Caputo derivative of a given function

$f(t)$, where the convergence order is $4 - \alpha$, which is higher than any reference available. Then we apply this scheme to Caputo type advection-dispersion equation. The convergence, stability, and error estimate for the Caputo type advection-dispersion equation are also given.

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MS96

Fractional Sturm-Liouville Theory for Spectral and Spectral Element Methods

We first introduce a new theory on fractional Sturm-Liouville problems, leading to the development of exponentially-accurate spectral and spectral element methods for time- and space-fractional PDEs. We introduce a new Discontinuous Petrov-Galerkin (DPG) method for fractional hyperbolic problems. Next, we present a unified Petrov-Galerkin (PG) spectral method for low-to-high dimensional fractional advection, diffusion, and Poisson/Helmholtz problems. We conclude the talk with a fractional collocation spectral method for efficient treatment of nonlinear/multi-term FPDEs.

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MS97

z-Pares: A Complex Moment Based Hierarchical Parallel Eigensolver Package

We have developed a parallel software package for solving generalized eigenvalue problems which is named z-Pares. This software enables users to utilize a large amount of computational resources because of its hierarchical parallel structure. z-Pares implements the Sakurai-Sugiura method proposed in 2003. This method computes an eigensubspace using complex moments that are obtained by contour integral. Numerical experiments and performance evaluations using matrices from some practical applications are shown.

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MS97

Improved Convergence and Parallel Performances for the FEAST Eigensolver

A new numerical scheme is introduced for the symmetric FEAST algorithm. The approach combines the FEAST subspace iteration technique using the approximate spectral projector with a truncated series of expanding generated subspaces. This approach significantly improves the current performance capabilities and convergence efficiency of the solver. In particular, the approach allows to reduce considerably the number of linear systems to solve by contour integration and then optimize the need in parallel computing power.

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MS97

Compact Rational Krylov Methods for Solving Nonlinear Eigenvalue Problems

We present a new framework of Compact Rational Krylov (CORK) methods for solving the nonlinear eigenvalue problem (NLEP):

$$A(\lambda)x = 0.$$

In this framework, we generalize the linearization based methods for solving NLEPs by writing the different linear pencils in a similar form and exploiting the corresponding structure. The CORK family of rational Krylov methods also uses a generalization of the compact Arnoldi decomposition. In this way, the extra memory cost due to the linearization of the original NLEP is negligible.

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MS97

Preconditioning Subspace Iteration for Large Eigenvalue Problems with Automated Multi-Level Sub-Structuring

The subspace iteration method (SIM) is a numerical procedure for normal mode analysis which has shown to be robust and reliable for solving very large general eigenvalue problems. Although its classical form as introduced by Bathe in the seventies of the last century is less efficient than the Lanczos iteration method in terms of CPU time, it is beneficial in terms of storage use if a very large number (say hundreds) of eigenmodes are needed and good approximations to the wanted eigenvectors are at hand. In this paper we take advantage of the automated multi-level sub-structuring (AMLS) to construct an accurate initial subspace for SIM. Along with the AMLS reduction we derive a very efficient preconditioning method for SIM which solves the linear systems for a transformed system with block diagonal system matrix whereas the multiplication with the mass matrix is executed in the original variables. The presentation is based on a joint paper with Pu Chen and Jiacong Yin, Peking University.

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MS98

Transport Properties of Periodic Metamaterials

Periodic microstructures such as metamaterials may contain arrays of nanowires, holes or metallic nanoparticles, whose material properties are complex-valued. Evaluation of their overall properties requires challenging computations. In this talk I will present a new approach based on the construction of periodic harmonic functions, and derive a formula for the effective tensor that excellently agrees with numerical calculations. Results of the talk has appeared in the Journal of Mathematical Physics 54, 053505 (2013).

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MS98

Homogenization for Sea Ice

Sea ice is a leading indicator of climate change, and a key component of Earth's climate system. As a material, sea ice is a porous composite of pure ice with submillimeter scale brine inclusions whose volume fraction and connectedness vary significantly with temperature. Fluid flow through the brine microstructure mediates a broad range of geophysical and biological processes. Sea ice also displays composite structures over much larger scales. For example, the sea ice pack itself is a fractal composite of ice floes and ocean, while surface ponds on melting Arctic sea ice exhibit complex dynamics and self-similar geometrical configurations. I will discuss how methods of homogenization and statistical physics are being used to study the effective properties of such systems. This work helps improve our understanding of the role of sea ice in the climate system, and the representation of sea ice in climate models.

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MS98

Review of Network Methods for Study of Singular Phenomena in Heterogeneous Media

This talk will provide a comprehensive overview of discrete network approximation techniques that have been demonstrated to be an elegant and powerful approach for deriving and justifying asymptotic formulas for (1) effective properties, (2) electric field, and (3) Dirichlet to Neumann map of high contrast disordered composites with inhomogeneities close to touching.

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MS98

On Global Microchannel Configurations for Liquid-Cooled Electronics Applications with Large Power Densities

We are interested in extending classical asymptotic approaches to allow for the spatial pattern wavenumber to vary on the macroscale variables and to find how changes in microstructure geometry affect macroscopic properties and transport. To this end, we consider the thermal transport of a fluid through nonuniformly spaced laminates, as a simple model for heat sinks in electronics. We find a coupled system of partial differential equations that describe the local microscale temperature and deviations from the Darcy pressure. Microscale values of all of these quantities are known in terms of the solutions to these effective eqautions. Examples of optimal channel geometries are found, which depend on the ability to transfer heat from the device to the enviornment, the orientation of the device with respect to gravity, and the available power needed to drive the fluid motion.

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MS99

Deterministic Quantities for Understanding Stochastic Dynamics

To understand dynamics under uncertainty, it is desirable to examine the quantities that carry dynamical information. A quantity called escape probability is investigated in order to describe transitions between dynamical regimes. This leads to consideration of a deterministic nonlocal partial differential equation. The speaker will focus on understanding stochastic dynamics by examining escape probability, in the context of prototypical examples in biophysical and physical settings. Relevant theoretical results will also be highlighted.

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MS99

A Multi-Time-Scale Analysis of Stochastic Chemical Reaction Network

We consider stochastic descriptions of reaction networks in which there are both fast and slow reactions, and the time scales are widely separated. We obtain a reduced equation on a slow time scale by applying a state space decomposition method to the full governing equation and describe our reduction method on the reaction simplex. We illustrate the numerical accuracy of the approximation by simulating several motivating examples.

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MS99

Fokker-Planck Equations for Stochastic Dynamical Systems with Symmetric Lévy Motions

The Fokker-Planck equations for stochastic dynamical systems, with non-Gaussian $\alpha-$stable symmetric Lévy motions, have a nonlocal or fractional Laplacian term. Taking advantage of the Toeplitz matrix structure of the time-space discretization, a fast and accurate numerical algorithm is proposed to simulate the nonlocal Fokker-Planck equations, under either absorbing or natural conditions.

The scheme is shown to satisfy a discrete maximum principle and to be convergent. It is validated against a known exact solution and the numerical solutions obtained by using other methods. The numerical results for two prototypical stochastic systems, the Ornstein-Uhlenbeck system and the double-well system are shown.

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MS99

DiPaola-Falsone Formula and Marcus Integral for Stochastic Dynamical Systems under non-Gaussian White Noise

DiPaola-Falsone formula is widely used in engineering and science. The equivalence between DiPaola-Falsone formula and Marcus integral was first proved by Sun, Duan and Li (arXiv:1202.2565 , Feb. 2012, the published final version appeared on Probabilistic Engineering Mechanics, Vol 32, pp:1-4, Jan. 2013). This talk further explores the relationship between DiPaola-Falsone formula and Marcus integral to solve some challenging problems associated with stochastic dyanamcial systems such as deriving Fokker-Planck equations and moment equations .

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MS100

Stable, Accurate, and Efficient Schemes for Parabolic Problems using the Method of Lines Transpose

We present a numerical scheme suitable for solving parabolic partial differential equations using the Method of Lines Transpose (MOL^T), and dimensional splitting. As a result, several one-dimensional boundary value problems can be solved in $O(N)$ work, to high precision; and a multi-dimensional solution is formed by dimensional sweeps. We prove that the scheme converges to prescribed orders in both time and space, and is L-stable. We demonstrate our solver on the Allen-Cahn equation, and discuss.

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MS100

Spectral Deferred Correction Methods for Vesicle Suspensions

Many fluid structure interaction problems have changing characteristic time scales throughout a simulation. For such problems, an adaptive high-order time integrator is important. Adaptive time stepping methods often require forming multiple numerical solutions to estimate the local truncation error. However, for vesicle suspensions, by taking advantage of the underlying physics, we are able to estimate the local truncation error with a single numerical solution. I will also show how we couple vesicle suspensions with spectral deferred correction methods in order to achieve high-order accuracy.

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MS100

Boundary Integral Methods for General Elliptic Problems

Elliptic problems such as Poisson, Yukawa, Helmholtz, Maxwell, Stokes and elasticity equations are converted to a consistent overdetermined first-order form. We derive simple well-conditioned integral equations for this form, analyze their solvability in Sobolev spaces, and build fast high-order solution methods with Ewald summation and the nonuniform fast Fourier transform.

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MS100

Volume Integral Equation Approaches for Fast Field Analysis in Inhomogeneous Media, with applications to MR Imaging and Induction Power Couplers

Volume integral methods are an appealing choice for computing electromagnetic fields in inhomogeneous media, such as a human head or an induction power coupler. These methods generates second-kind integral equations, so matrix-implicit iterative methods should convergence rapidly, though convergence is often slow in practice. In this talk we show that the observed slow convergence can be an artifact of mismatching the material and basis function boundaries, and resolve the mismatch to generate a fast FFT-accelerated iterative method suitable for MR imaging field computation. We also show an approach effective for induction power couplers, where proper boundaries allow the use of a numerically computed Toeplitz-Hankel decomposition.

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MS101

Computing Singular and Nearly Singular Integrals

We will describe recent progress with J. Wilson and W. Ying in computing a singular or nearly singular integral, such as a harmonic function given by a single or double layer potential on a smooth, closed curve surface in 3D. The present approach is suited for use with moving interfaces since the representation of the interface is simple and the value of the integral can be found at nearby points as well as on the surface. The value of the integral is found using a standard quadrature, with the singularity replaced by a regularized version. Correction terms are then added for the errors due to regularization and discretization. They are needed at points near the surface, since the integrals are nearly singular. Surface integrals can be computed in overlapping coordinate grids; however, in recent work, we improve this method and make it more practical. We use a technique of J. Wilson for surface integration which allows accurate representation without explicit reference to the coordinate charts. For efficient summation, we use a treecode developed by Duan and Krasny for the Gaussian regularization of the fundamental solution of Laplacian.

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MS101

An Interface Problem for Biomolecules

A biomolecule placed in solvent can be viewed as generating an interface separating the biomolecule and vacuum from the surrounding solvent. The size and configuration of this interface plays an important role in biomolecule functions such as protein folding and docking. We develop the setup and algorithms to capture such interfaces, using a variational framework and gradient descent flow for energy minimization; the level-set method to handle interfacial motion and topological changes; and a new finite difference compact stencil approach to compute electrostatic contributions.

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MS101

An Overlapping Patch Boundary Integral Method for Dynamic Interface Problems

A nonstiff boundary integral method for 3D interfacial flow with surface tension or elastic membrane stress is presented. The stiffness is removed by developing a small-scale decomposition, based on a generalized isothermal parameterization of the interface. New applications of the method to water waves and hydroelastic waves will be discussed. We will also present preliminary work on a new version of the method which uses domain decomposition or overlapping coordinate patches to describe the interface. This is necessary to treat problems for which generalized isothermal coordinates do not provide a global parameterization. It also provides a framework for significant spatial adaptivity of the method. This is joint work with David Ambrose and Carlo Fazioli.

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MS101

A Kernel-Free Boundary Integral Method for Moving Interface and Free Boundary Problems

The kernel-free boundary integral method is a Cartesian grid-based boundary integral method for elliptic partial differential equations. The method avoids direct evaluation of boundary integrals and does not need to know an analytical expression for kernels of boundary integrals or the fundamental solution of the associated elliptic partial differential equation. To evaluate a boundary integral, the kernel-free boundary integral method first solves an equivalent interface problem on a Cartesian grid and then interpolates the grid solution to get values of the corresponding boundary integral at discretization points of the boundary or interface of the problem. The method is efficient as well as accurate. Numerical experiments for some moving interface and free boundary problems such as the Hele-Shaw flow will be presented in this talk.

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MS102

Elastic Structure Coupled with the Air/water Interface, Inspired by Diving Birds

We investigate how a soft elastic body responds to water-entry impact analogous to a bird diving into water to catch prey. Experimentally, dumbbell shaped objects made of two acrylic spheres connected by an elastic rod are dropped into water. A buckling threshold was calculated using a linear Euler beam theory, which is expressed in terms of body geometry, impact force, and elastic rod stiffness. This threshold may have implication as to how birds are able to safely dive into water at high speeds and avoid any neck-injury.

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MS102

Simulations of Pulsating Sessile Coral and the Resulting Fluid Flow

Soft coral of the family Xeniidae have a pulsating motion, a behavior not observed in other immobile marine organisms. These pulsations consume a large amount of energy, and determining the benefits of this behavior is vital to understanding the evolution of such animals. We will present direct numerical simulations of the pulsations of the coral and the resulting fluid flow by solving the Navier-Stokes equations coupled with the immersed boundary method to model individual and interacting polyps.

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MS102

Performance of Vortex-Based Propulsion on a Jellyfish-Like Swimmer

This study develops a computational approach to investigate the vortex wakes generated by an axisymmetric jellyfish-like swimmer. The parameter space of swimmer body kinematics is explored. The effects of these parameters on thrust, input power and circulation are quantified. Two metrics, cruising speed and energy cost of locomotion, are used to evaluate the propulsion performance. The knowledge from this study can be used for the design of robotic swimmers that use vortex rings for propulsion.

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MS102

Simulation of a 3D Viscous Flow Past a Deformable Thin-Walled Circular Disk Tethered at Its Center by An IB Method

Motived by animal locomotion in a fluid, we model and simulate the interaction of a viscous incompressible flow past a deformable circular thin-walled disk tethered at its center. The thin-walled structure is modelled by a classic approach (shell as an assembly of plate elements) and a special finite element method (the corotational scheme) is used to solve numerically the partial differential equations (PDE) governing the motion of the thin-walled structure. The flow is modelled by the classic viscous incompressible Navier-Stokes equations and are solved numerically by a popular lattice Boltzmann model (D3Q19). The interaction between the structure and flow is handled by the immersed boundary (IB) method. Our simulations have identified three distinct deformation modes of the thin disk: circular, folding, and triple-petalled, depending on the parameters of the flow and the structure. Our results are in very good agreement with laboratory experiments published very recently (L Schouveiler and C Eloy, Flow-induced drapping, Phys Rev Lett 111: 064301, 2013).

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MS103

Multiple Scattering Using the Generalized Foldy-Lax Formulation

Consider the scattering of a time-harmonic plane wave incident on a two-scale heterogeneous medium, which consists of scatterers that are much smaller than the wavelength and extended scatterers that are comparable to the wavelength. This talk will present the computational study for the wave propagation. The imaging functions are designed to visualize the location of the point scatterers and the shape of the extended obstacle scatterers.

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MS103

Fast Solver for Multi-Particle Scattering in a Layered Medium

This talk is devoted to the scattering of multi-particle in a layered medium. Assume the medium has three layers and a large number of dielectric particles are randomly distributed and well separated in the middle layer. The size of each particle is comparable to the wavelength and the shape of each particle is the same up to a rotation but not restricted to be a disk. The field is excited by some external source. Direct evaluation for the scattered field is notoriously slow due to the large number of unknowns. We propose a method based on the combination of Sommerfeld integral, scattering matrix and fast multiple method(FMM), which can dramatically speed up the calculation. Numerical experiments will be shown to confirm the efficiency. This is a joint work with Leslie Greengard and Motoki Kobayashi.

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MS103

The Factorization Method for a Cavity in An Inhomogeneous Medium

We consider the inverse scattering problem for a cavity that is bounded by a penetrable anisotropic inhomogeneous medium of compact support and seek to determine the shape of the cavity from internal measurements on a curve or surface inside the cavity. We derive a factorization method which provides a rigorous characterization of the support of the cavity in terms of the range of an operator which is computable from the measured data. The support of the cavity is determined without any a-priori knowledge of the properties of the surrounding anisotropic medium. Numerical examples are given showing the viability of our method.

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MS103

Surface Plasmon Enhancement in Nano Dielectric Layer

We consider the experiments done by Brian Cullum and his group at UMBC of multilayer silver film over nanostructure substrates that provide much greater surface-enhanced Raman scattering signal compared to single layer of silver with the same thickness as multilayer. We are going to discuss the multilayer and nano gap effects mathematically in an experimental related set up and compare the results with that of the experiments.

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MS104

Improving Computing Skills of STEM Graduates

Computing skills are today a requirement for any STEM graduate, yet we still have not found a way to embed computing throughout the curriculum in engineering and mathematics. Many students only experience an "introduction to programming" class in their freshman year, and then we expect them to teach themselves whatever they might need to succeed in other courses, and in their careers. It's no wonder that so many scientist and engineers don't use best practices for scientific computing, including good software design and development, reproducibility, testing and ensuring the permanence of the scientific evidence they create. A few trends are taking hold that have potential to improve this situation. Efforts like Software Carpentry (Mozilla Foundation) are spreading best practices in software creation and curation: version control, testing, automation, provenance, sharing. Less commonly, some schools are revising their approach to computing in the curriculum. We are conducting a pilot study using just-in-time online modules that teach context-based computing for engineers. The context-based approach has already demonstrated its effectiveness, e.g., in the media computing course introduced at Georgia Tech some years back (which not only improved student success, but also reduced the gender achievement gap in computing). We are extending this approach with the just-in-time delivery of skills, as a "performance support" device. In this talk, we will present our theory of action for this educational intervention, the design concepts, and the preliminary data from our evaluation.

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MS104

Towards Verifiable Publications

Research papers provide the primary mechanism for sharing novel methods and data. Papers describe experiments involving small amount of data, derivations on that data, and associated methods and algorithms. Readers reproduce the results by repeating physical experiments, performing hand calculations, and setting forth logical arguments. The scientific method in this decade has become decisively computational, involving large quantities of data, complex data manipulation tasks, and large, and often distributed software stacks. The research paper, in its current text form, is only able to summarize the associated data and computation and not able to reproduce it computationally. While papers corroborate descriptions through indirect means, such as by building companion websites that share data and software packages, these external websites continue to remain disconnected from the content within the paper, making it difficult to verify claims and reproduce results. There is a critical need for systems that minimize this disconnect. We describe Science Object Linking and Embedding (SOLE), a framework for creating verifiable publications by linking them with associated science objects, such as source code, datasets, annotations, workflows, re-playable packages, and virtual machine images. SOLE provides a suite of tools that assist the authors to create and host science objects that can then be linked with research papers for the purpose of assessment, repeatability, and verification of research. The framework also creates a linkable representation of the science object with the publication and manages a bibliography-like specification of science objects. In this presentation, we will introduce SOLE through examples from climate science, chemistry, biology, and computer science, and describe its use for augmenting the content of computation-based scientific publications.

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MS104

What Is Worth Reproducing in Computational Science?

What is driving the call for reproducible science? The sentiment is that the archival literature should have a reproducible basis and computational science is particularly ephemeral due to the ever-changing landscape of computation. Simultaneously, we see an explosion of papers that exceeds the ability of scientists to keep up with. Should we add to this tsunami of data with reproducibility? Perhaps reproducibility will stem the tide and make the literature more compact and valuable.

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MS104

Constructing Guaranteed Automatic Numerical Algorithms for Univariate Integration

The project establishes an automatic, adaptive algorithm for solving univariate integration problems using trapezoidal rule. The algorithm provides rigorous guarantees of success and computational cost. The key idea is that the error analysis should be done for cones of input functions rather than balls. Theoretical and numerical results are provided.

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MS105

A Practical Guide to Measure-Theoretic Inversion: Algorithms and Error Estimation

We describe the practical elements of a measure-theoretic framework for solving stochastic inverse problems for deterministic models with uncertain parameters. Theoretical results on the existence and uniqueness of solutions are presented that outline a basic computational algorithm for approximation of solutions. We extend the algorithm for estimating solutions in high dimensional parameter spaces and explore an a posteriori error analysis on computed probabilities of events.

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MS105

Spatially Heterogeneous Parameter Estimation Within the Advanced Circulation (ADCIRC) Model

We describe a framework for estimating spatially heterogeneous paramters critical to the accuracy of model forecasts of storm surge. We use pixelated land cover data to determine the spatial distribtion of land cover classifications which we consider certain. We estimate the Manning's n (a bottom friction paramter) value associated with these land cover classifications. We solve an inverse problem for these values using a measure-theoretic approach applied to the ADCIRC storm surge model.

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MS105

Uncertainty Quantification and Parameter Estimation for Groundwater Contaminant Transport

The movement of contaminant plumes in underground aquifers is highly dependent on many hydrogeological parameters. It is often prohibitively expensive or impossible to make accurate and reliable measurements of these parameters in the field. We utilize a measure-theoretic inverse framework to perform uncertainty quantification and estimation for these parameters. Forward problem calculations of quantities of interest are improved using a posteriori error estimates calculated by solving adjoint problems.

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MS105

Advanced Coastal/Subsurface Models and a Measure-Theoretic Uq Framework Using Real Data

In this talk we'll focus on advanced models for near shore flows and multiphase flows in the subsurface. In particular, the focus will be on identifying the computational issues that need to be addressed in estimating parameters especially in highly heterogeneous materials in the case of subsurface flows. We will also describe methods of dealing with real data to quantify uncertainties.

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MS106

Novelty, Convention and Scientific Impact

Analyzing all 17 million papers in the Web of Science database, we employ a methodology based on journal pairings that characterizes each paper by the convention and novelty of the prior work combined. We measure the relative conventionality and novelty of the prior work that a paper combines by examining the journals referenced.

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MS106

Modeling the Dynamics of Vector-Host Interaction of Easter Equine Encephalitis

Eastern equine encephalitis (EEE) virus is a highly pathogenic mosquito-borne infectious disease that is responsible for outbreaks in humans and equines, resulting in high mortality or severe neurological impairment in most survivors. In the northeastern United States, EEE virus is maintained in an enzootic cycle involving the mosquito, Culiseta melanura, and perching birds in freshwater swamp habitats. Utilizing the SIR model, we examine the influence of the different bird species and time of year in the spread and survival of EEE.

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MS106

Controllability Of Infections In Models Exhibiting Multiple Endemic Equilibria

In mathematical infectious disease epidemiology, reducing R_0 to slightly below 1 is sufficient to control the infection under consideration. This is true only if the model doesnt show the existence of endemic equilibria for $R_0 < 1$. However, some models of infections exhibits backward bifurcation or even hysteresis. In this case reducing R_0 to below 1 is necessary but not sufficient to eliminate the infection. We show a family of models showing hysteresis and find the conditions on model parameters assuring the elimination of the infection.

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MS106

Modeling the Transmission Dynamics of H7N9 Avian Influenza Outbreak: Poultry Markets

The outbreak of H7N9 avian influenza in humans in Asia during 2013 and 2014 underlines the need for better understanding of the mechanisms by which avian influenza spreads among bird flocks in live markets. Here we employ and susceptible, exposed, infected, recovered (SEIR) model and fit the parameters of the model to low-pathogenic avian influenza prevalence data collected in in Hong Kong live bird markets between 1999 to 2005. In conjunction with climate data from the Hong Kong observatory, we examine the dependence of model parameters on temperature, relative humidity, and absolute humidity.

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MS108

Comparison and Integration of Genomic Profiles Predict Brain Cancer Survival and Drug Targets

Recently, we demonstrated the effectiveness of the GSVD in comparing patient-matched genomic profiles and identifying a pattern of DNA copy-number aberrations that correlates with glioblastoma survival. Here, we show cross-platform validation of this signature, bringing it a step closer to the clinic. Surprisingly, we also find that the prognostic value of the signature is maintained for lower-grade astrocytomas (LGAs). GSVD of LGA patient-matched profiles uncovers molecular similarities and differences between glioblastoma and LGA that suggest drug targets.

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MS108

Network-Based Methods for Understanding Disease and Predicting Therapy

Cellular processes are driven by complex interacting networks comprised of diverse cellular components. Although we have seen a revolution in our ability to generate multiomic data, our ability to use these data to infer informative cellular networks has lagged. We will present data-driven methods that incorporate knowledge about potential network structure that capture essential network features, leading to clinically-relevant insight into disease processes.

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MS108

Variant Prioritization by Genomic Data Fusion

Exome sequencing has revolutionized the discovery of mutations causing rare monogenic disorders. However, sequencing identifies many candidate mutations and we need better methods to prioritize variants for validation. Our methodology for genomic data fusion uses machine learning to integrate multiple strategies to detect deleteriousness of mutations. Our key innovation is the incorporation of a computational method for gene prioritization, which scores mutated genes based on their similarity to known disease genes.

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MS108

Discovery of Multidimensional Modules in Cancer Genomic Data

Recent technology has made it possible to simultaneously perform multi-platform genomic profiling of biological samples, resulting in so-called multidimensional genomic data. Such data provide unique opportunities to study the coordination between regulatory mechanisms on multiple levels. However, integrative analysis of multidimensional genomics data for the discovery of combinatorial patterns is currently lacking. Here, we develop a series of methods to address this challenge. We applied this method to data from The Cancer Genome Atlas, and prove its utilities in identifying subtly perturbed cancer pathways and distinguishing patients with different survival time.

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MS109

The Role of Numerical Boundary Procedures in the Stability of Perfectly Matched Layers

We address the temporal energy growth associated with numerical approximations of the perfectly matched layer (PML) for Maxwell's equations in first order form. In the literature, several studies have shown that a numerical method which is stable in the absence of the PML can become unstable when the PML is introduced. We demonstrate in this talk that this instability can be directly related to numerical treatment of boundary conditions in the PML. At the continuous level, we establish the stability of the constant coefficient initial boundary value problem for the PML. To enable the construction of stable numerical boundary procedures, we derive energy estimates for the variable coefficient PML. Numerical experiments verify the theoretical results

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MS109

A Fast Algorithm for 3D Azimuthally Anisotropic Velocity Scan

Conventional velocity scan can be computationally expensive for large-size seismic data, particularly when the presence of anisotropy requires multiparameter scanning. We introduce a fast algorithm for 3D azimuthally anisotropic velocity scan by generalizing the previously proposed 2D butterfly algorithm for hyperbolic Radon transform. To compute semblance in a two-parameter residual moveout domain, the numerical complexity of our algorithm is roughly $O(N^3 \log N)$ as opposed to $O(N^5)$ of the straightforward velocity scan, with N being the representative of the number of points in either dimension of data space or parameter space. Synthetic and field-data examples demonstrate the superior efficiency of the proposed algorithm.

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MS109

Uncertainty Quantification for Large-Scale Bayesian Inverse Problems with Application to Ice Sheet Models

Modeling the dynamics of polar ice sheets is critical for projections of future sea level rise. Yet, there remain large uncertainties in the basal boundary conditions employed within ice sheet models, which rely on the incompressible Stokes equations with shear thinning rheology to describe the behavior of ice sheets. We address the problem of quantifying uncertainties in the inference of basal boundary conditions for large-scale ice sheet inverse problems within the framework of Bayesian inference.

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MS110

Bio-inspired Wing Design for Flying Micro Robots

Low Reynolds number aerodynamics is of great importance for the optimization of Micro Air Vehicles (MAV). A possibility to improve the flight performance of MAVs is to take inspiration from efficient flyers and swimmers in nature. Studies have shown that the scales on the wing of a butterfly as well as the ribs present on the dermal denticles of sharks can have a positive effect on the fluid dynamic performance, using different principles of flow boundary layer control which increase the lift to drag ratio. In this talk, I will present different fabrication methods for mimicking the scales on the wings of butterflies as well as the ribs present on the skin of sharks. Furthermore, I will present recent work on high-performance butterfly-inspired wing shapes that can be used for MAVs and I will outline how optimized wing designs in robotics can give insights to questions in evolutionary biology.

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MS110

Sharks and Butterflies: Micro-Sized Scales Have Macro Effects

Sharks and butterflies swim and fly in two completely different flow regimes, yet the structure of their surfaces interacting with the surrounding fluid look amazingly similar. Both are not smooth but have unique microgeometries that potentially work to control the flow. Sharks have moveable scales that appear to act as a passive, flow-actuated dynamic roughness for separation control. Alternatively, butterfly scales appear to fundamentally alter the local skin friction drag depending on flow orientation.

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MS110

Friction Enhancement in Snake Locomotion

Snakes are one of the worlds most versatile organisms, at ease slithering through rubble or climbing vertical tree trunks. In this study, we elucidate the physics of snake interactions with its complex environment. We present a series of experiments and supporting mathematical models demonstrating how snakes optimize their speed and efficiency by adjusting their frictional properties as a function of position and time. We use this discovery to build two snake-robots with enhanced climbing capabilities.

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MS110

Bioinspired Transformative Skins: From Fundamental Physics to Applications

As human beings age, our skins develop wrinkles and folds an undesirable feature that has fueled a multi-billion-dollar skin care industry. Conversely, many animals such as cephalopods can reversibly create skin patterns to match surrounding textures for active camouflage. This talk will present a unified model that can predict various modes of instabilities and patterns on skins. We will then discuss novel transformative applications of surface instabilities such as tunable superhydrophobicity and on-demand stem-cell alignment by seeking bioinspirations.

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MS111

A Nonlinear QR Algorithm for Unstructurally Banded Nonlinear Eigenvalue Problems

A variation of Kublanovskaya's method for solving nonlinear eigenvalue problems will be presented for the case of unstructurally banded problems. The new method is iterative and specifically designed for problems too large to use dense linear algebra techniques. A new data structure will also be presented for storing the matrices to keep memory and computational costs low. In addition, an algorithm will be presented for computing several nearby eigenvalues to already computed eigenvalues.

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MS111

High-Performance Algorithms for Computing Pseudospectra

While numerous authors investigated parallel schemes for computing pseudospectra over the past two decades, no technique has yet emerged as a massively-parallel blackbox replacement for Liu's algorithm, which uses the shifted Schur factor to drive inverse iteration. This talk proposes and evaluates two classes of distributed-memory algorithms which interleave many Lanczos processes in order to greatly increase efficiency relative to traditional schemes: (1) Schur decomposition followed by simultaneous shifted triangular solves, and (2) reduction to Hessenberg form followed by simultaneous shifted Hessenberg solves. While the underlying high-performance computational kernels of these two inverse iteration procedures were proposed nearly two decades ago by Henry in the context of control theory, they seem to be underappreciated by the pseudospectra community.

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MS111

An Indefinite Variant of LOBPCG for Definite Matrix Pencils

We propose a novel preconditioned solver for generalized Hermitian eigenvalue problems. More specifically, we address the case of a definite matrix pencil $A - \lambda B$ (i.e., A, B are Hermitian and there is a shift λ_0 such that $A - \lambda_0 B$ is definite). Our new method is a variant of the popular LOBPCG method operating in an indefinite inner product. It also turns out to be a generalization of the recently proposed LOBP4DCG method for solving product eigenvalue problems.

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MS111

Preconditioned Locally Minimal Residual Methods for Large-Scale Eigenproblems

We study the preconditioned locally minimal residual method (PLMR) for computing invariant pairs of nonlinear eigenproblems of the form $T(\lambda)v = 0$. PLMR is a newly-developed preconditioned eigensolver which does not require the computation of shift-invert matrix vector products. It bears close connections to several well-known algorithms, including LOPCG, Jacobi-Davidson and the inverse-free preconditioned Krylov subspace method. Numerical experiments show the flexibility and competitiveness of PLMR on large-scale benchmark nonlinear eigenproblems.

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MS112

Multiscale 3D Simulation of Whole Blood in Complex Geometry

A 3D multiscale immersed-boundary method is developed to simultaneously simulate major hemodynamics processes in whole blood flowing in microvascular network. The whole blood is represented as a suspension of red blood cells, white blood cells and platelets. The dynamics of each cell is resolved using a front-tracking method. The vascular network in 3D is modeled directly using a ghost-node immersed-boundary method. The method simulates interaction among blood cells, platelet adhesion, WBC rolling adhesion, and dispersion of drug-carriers in vascular network.

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MS112

Simulation of Cellular Blood Flow in Microvessels

The cellular character of blood leads to complex flow phenomenology in vessels of comparable size to the blood cells. We have designed a fast spectral boundary integral algorithm that simultaneously solves for the dynamics of the highly deformable blood cells and their flow in such configurations. The talk will include an outline this method and discussion of two applications: the transport of magnetic nanoparticles amongst the flow blood cells the flow of red-blood cells through a model spleenic slit.

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MS112

Long-Wave Dynamics of An Inextensible Plannar Membrane in An Electric Field

We investigate the long-wave nonlinear dynamics of an inextensible capacitive elastic membrane under ac and dc electric fields. In the lubrication framework we derive a nonlinear evolution equation for the membrane height with an integral constraint. Different membrane dynamics, such as undulation and flip-flop are found at different electric field strengths and membrane area. In particular an alternating wave on the membrane is found as a response to an ac field in the perpendicular direction.

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MS112

Extensional Dynamics of Vesicles: Asymmetric Rayleigh-Plateau, Burst, and Pearling

When deformable vesicles with an aspect ratio of at least 3.5 are subject to extensional flow, they undergo an elongational transition above a critical capillary number. We complete 3D boundary integral simulations and develop a multipole expansion spectral theory for vesicles with aspect ratios up to 10. We demonstrate that the critical conditions can be predicted quantitatively. Moreover, a second burst transition at higher Capillary number which is a prelude to pearling is demonstrated.

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MS113

A Difference Equations Approach to Studying Oscillations in a Suspension Bridge involving a Nonlinear Cable Function

In their 2000 paper 'Multiple Periodic Solutions to a Suspension Bridge Ordinary Differential Equation', P. J. McKenna and K. S. Moore studied oscillations in a suspension bridge by analyzing periodic solutions to the system of nonlinear ordinary differential equations

$$\begin{aligned} \theta' &= -\frac{6K}{m}\cos\theta\sin\theta - \delta_1\theta' + f(t) \\ y' &= -\frac{2K}{m}y - \delta_2 y' + g \end{aligned} \tag{3}$$

where δ_1, δ_2 are damping constants, K, m are positive parameters, g is the force due to gravity and $f(t)$ is an external force at time t. They used Leray-Schauder Degree Theory along with numerical methods like the Runge-Kutta Method to do so. In this talk, I will analyze the periodic solutions of (1) using a slightly newer more nontraditional method. More specifically, I will introduce a *nonlinear cable function* $c(t)$ in the y'-equation in (1), discretize the resulting system into a system of two coupled second-order second-degree difference equations and then perform a local and global stability analysis of this new system using the mathematical theory of difference equations. One of the biggest challenges of this study will be setting up the global analysis framework for general second-order second-degree difference equations along the way since this topic is still largely an open research area. However if successful, this study will provide a way to analyze the local and global dynamics of periodic solutions of (1) for entire regions of initial conditions *and* parameter values as opposed to a limited number of initial conditions and parameter values as is generally possible using numerical methods.

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MS113

From Billiard Dynamics to Thermodynamics

We develop a stochastic approach to thermodynamics using a model of gas-surface interactions derived from a randomized version of billiard dynamical systems. We first recover some classical results from the kinetic theory of gases, specifically Knudsen's Law for angle of reflection. We then derive diffusion constants for particles moving in a channel with rough walls. Finally, we develop notions of temperature, heat flow, and entropy production, leading to models of simple machines.

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MS113

Predictor-Based Tracking for Neuromuscular Electrical Stimulation

Neuromuscular electrical stimulation is a technology that helps restore functionality to human limbs. We study neuromuscular electrical stimulation of the human knee, by providing a tracking controller such that the tracking error globally asymptotically converges to zero, under any input delay, a state constraint on the knee position, and sampled state measurements. We use a new method for constructing predictors. This work is joint with Iasson Karafyllis, Marcio de Queiroz, Miroslav Krstic, and Ruzhou Yang.

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MS113

Solving Linear Differential Equations and Inverting Matrices: Key Formulas

In preparing a new textbook on *Differential Equations and Linear Algebra*, one function and one formula took a central place: the solution $g(t)$ with driving function $\delta(t)$ = impulse response = Green's function = fundamental solution. When the driving function is $f(t)$, the solution is the integral of $g(t-s)f(s)$. The talk will connect the different ways to find this growth factor $g(t)$. Separately we call attention to an amazing expression for A^{-1} when that matrix is tridiagonal.

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MS114

Boundary Integral Equation for an Ion Channel in Electrolyte Media

In this talk, computation of the electrostatic potential arising from the hybrid solvation model for ion channels will be discussed. The Poisson-Boltzmann (P-B) equation is considered. In order to model the cell membrane where the ion channel is located, the layered media Green's function of the P-B equation is used to develop a boundary integral equation for a finite hight hollow cylinder. Two fictitious half spheres are attached top and bottom of the cylinder to avoid edge singularities. Then, a body-fitted mesh is used to discretize the boundary of the cylinder. Several numerical examples will be presented.

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MS114

Life after Sweeping: Hopping for the Helmholtz Equation

The high-frequency 3D Helmholtz equation in a heterogeneous medium is a difficult question in numerical analysis. Direct solvers are either unwieldy to set up for the problem as a whole, or are hard to link up in a domain decomposition framework. In this work we consider an upwind, incomplete form of Green's identity as a high-quality transmission boundary condition, and use it to define polarized waves at interfaces between subdomains. This approach is attractive when local Green's functions are precomputed, and a fast algorithm is available for their application: we obtain an algorithm with complexity sublinear in the number of unknowns normally needed to represent the solution in the volume. The new method can be seen as a generalization of the sweeping preconditioner of Engquist-Ying to larger subdomains. Joint work with Leonardo Zepeda-Nunez.

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MS114

A Robust Maxwell Solver in Axisymmetric Geometries

Several integral equations used for electromagnetic scattering problems suffer from instabilities at low frequencies. Some instabilities occur from purely numerical considerations, others from non-trivial topology of the scatterer. In this talk, we review an integral equation formulation based on generalized Debye sources which addresses both of these forms of low-frequency breakdown. We will present a high-order solver based on this formulation for axisymmetric geometries, both for perfect conductor and dielectric problems.

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MS114

Scalable Quasi-direct Solvers for 3D Elliptic Problems

While scalable distributed-memory techniques have recently been proposed for the approximate factorization of $HSS/H^2/H$-matrices defined through a "weak" admissibility condition, no scalable $HSS/H^2/H$-matrix factorization strategy is known which can handle the "strong" admissibility condition needed to represent Green's functions of 3D elliptic problems. This talk evaluates two directions for circumventing this problem: (1) an approximate Newton-Schulz iteration based upon a new parallelization of H-matrix/H-matrix multiplication and (2) the recently introduced Hierarchical Interpolative Factorization.

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MS115

A Treecode-Accelerated Boundary Integral Poisson-Boltzmann Solver for Solvated Proteins

We present a treecode-accelerated boundary integral (TABI) solver for electrostatics of solvated proteins described by the linear Poisson-Boltzmann equation. The integral equations are discretized by centroid collocation. The linear system is solved by GMRES and the matrix-vector product is carried out by a treecode. We compute the electrostatic solvation energy for a protein. We compare TABI results with those obtained using the grid-based APBS code and we present parallel TABI simulations.

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MS115

A Hybrid Immersed Boundary and Immersed Interface Method for Two-Phase Electrohydrodynamic Simulations

In this talk, we introduce a hybrid immersed boundary (IB) and immersed interface method (IIM) to simulate the dynamics of a drop under the influence of electric field in Navier-Stokes flows. Instead of applying the volume electric force arising from the Maxwell stress tensor, we alternatively treat the electric effect as an interfacial force bearing the normal jump of Maxwell stress on the interface. A series of numerical tests with different permittivity and conductivity ratios are performed and compared with the results obtained by the small deformation theory.

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MS115

Electro-Hydrodynamics of Vesicle Suspensions

We investigate the mechanics of inextensible capacitive elastic membranes in applied electric fields. A new boundary integral formulation for the coupled electric and hydrodynamic governing equations will be presented. The membrane evolution is characterized by a competition between elastic energy, inextensibility, non-local hydrodynamic interaction, electric potential and the a.c. field field frequency. We will discuss new insights gained via numerical simulations.

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MS115

Recent Developments of Grid Based Particle Method

Grid based particle method (GBPM) is a meshless point method for moving interface problems. GBPM has a particle method nature which can capture a moving interface accurately and efficiently. At the same time these meshless particles carry both Lagrangian and Eulerian information simultaneously with the help of a underlying grid which allows one to handle different kind of topological changes easily. Also adaptivity can be incorporated into GBPM naturally. In this presentation, I will talk about some recent developments in GBPM and using it to model various moving interface problems.

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MS116

Ten Good Reasons for using Kernel Reconstructions in Adaptive Finite Volume Particle Methods

This talk discusses the utility of meshfree kernel techniques in adaptive finite volume particle methods (FVPM). To this end, we give ten good reasons in favour of using kernel-based reconstructions in the recovery step of FVPM, where our discussion addresses relevant computational aspects concerning numerical stability and accuracy, as well as more specific points concerning efficient implementation. Special emphasis is finally placed on more recent advances in the construction of adaptive FVPM, where WENO reconstructions by polyharmonic spline kernels are used in combination with ADER flux evaluations to obtain high order methods for hyperbolic problems.

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MS116

Model Selections for Polynomial Kernel Regressions

Polynomial kernel regression is one of the most commonly used methods in numerical analysis and statistics. However, in dealing with many real world problems, choosing the right degree of a polynomial kernel is a challenging issue, as poor choices often lead to either "under-fitting" or "over-fitting". We propose and study criteria and new strategies especially designed for this purpose. We provide both theoretical analysis and numerical simulations to illustrate the performance of the new strategies.

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MS116

Multiscale Rbf Interpolation and Collocation

The combination of compactly supported radial basis functions with a residual correction scheme has proven to be numerically extremely efficient and accurate for solving both scattered data interpolation and collocation problems. In this talk I will give a short survey of what is known so far and address recent developments particularly when it comes to solving partial differential equations. For example, I will address adaptivity, boundary conditions and scaling.

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MS117

Conjugate Gradient Iterative Hard Thesholding

Conjugate Gradient Iterative Hard Thresholding is a greedy algorithm for solving the compressed sensing and matrix completion problems combining the advantages of the low per iteration complexity of Normalized Iterative Hard Thresholding and the effectiveness of projection based algorithms such as Hard Thresholding Pursuit and Compressive Sampling Matching Pursuit. This talk will also introduce the compressed sensing and matrix completion problems as examples of low dimensional models.

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MS117

Denoising Simultaneously Structured Signals

Models or signals exhibiting low dimensional behavior (e.g., sparse signals, low rank matrices) arise in many applications in signal processing and machine learning. We focus on models that have multiple structures simultaneously; e.g., matrices that are both low rank *and* sparse, arising in phase retrieval, quadratic compressed sensing, and cluster detection in social networks. We consider the estimation of such models from direct observations corrupted by additive Gaussian noise. Our main result is to provide tight upper and lower bounds on the mean squared error (MSE) of a *convex* denoising program that uses a combination of regularizers to induce multiple structures. In the case of low rank and sparse matrices, we quantify the gap between the MSE of the convex program and the best achievable error, and also compare it with a simple nonconvex thresholding algorithm in a certain regime of signal-to-noise ratio.

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MS117

Frontiers of Atomic Norm Minimization

We often model signals from the physical world with continuous parameterizations. Unfortunately, continuous models pose problems for the tools of sparse approximation, and popular discrete approximations are fraught with theoretical and algorithmic issues. In this talk, I will propose a general, convex-optimization framework—called atomic-norm minimization—-that obviates discretization and gridding by generalizing sparse approximation to continuous dictionaries. I will discuss recent theoretical and algorithmic advances that demonstrate the utility of this framework in a diverse set of applications.

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MS117

Modal Analysis with Compressive Measurements

We consider the problem of determining the mode shapes of a structure from a compressed collection of vibrational time series recordings, as might be collected by a network of wireless sensor nodes performing Compressive Sensing (CS). We consider three different CS strategies, analyze a simple SVD-based method for estimating the mode shapes from compressive samples without performing CS reconstruction, and provide novel finite sample reconstruction bounds. This work has potential applications in structural health monitoring.

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MS118

Universe Geometry

This brief history will elucidate the role of supercomputers in enhancing progress in mathematics. Moving through the exciting history of supercomputing, we will broach the top supercomputers of its time and its important applications. This will be followed by a stimulating story about a supercomputer simulation that has proven the validity of a theory that was proposed 40 years ago for the evolution of the universe.

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MS118

Understanding the Universe with Petascale Simulations - the Enzo Cosmology Code

Abstract not available at time of publication.

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MS118

Talk title: Creating a Virtual Universe

Abstract not available at time of publication.

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MS119

Irregular Polyomino Tiling via Integer Programming with Application in Phased Array Antenna Design

A polyomino is a generalization of the domino and is created by connecting a fixed number of unit squares along edges. Tiling a region with a given set of polyominoes is a hard combinatorial optimization problem. This work is motivated by a recent application of irregular polyomino tilings in the design of phased array antennas. Exact, approximate, and heuristic solution methodologies are proposed. Encouraging computational results including phased array antenna simulations are reported.

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MS119

Accelerated Bregman Operator Splitting with Variable Stepsizes

In this talk, we present a novel scheme, namely accelerated Bregman operator splitting with variable stepsize (ABOSVS), for solving problems of the type $\min\{1/2||Au-f||_2^2 + \phi(Bu)\}$, where ϕ may possibly be nonsmooth. Our proposed algorithm incorporates a multi-step acceleration scheme into BOSVS to improve the convergence rate. ABOSVS is compared with other state-of-art algorithms by using partially parallel magnetic image reconstruction. The numerical results show that the proposed ABOSVS algorithm performs more efficiently in terms of image quality and CPU time.

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MS119

Accelerated First-Order Method for Convex Composite Optimization and the Applications in Image Analysis

We present an accelerated scheme for solving a class of convex composite optimization problems and its application in image analysis. The proposed AL-ADMM method, namely accelerating linearized alternating direction method of multipliers, has accelerated rate of convergence in terms of its dependence on Lipschitz constant of the smooth component. A backtracking technique for searching Lipschitz constant is also proposed for practical performance.

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MS119

Image Reconstruction for Dynamic Cone Beam Computed Tomography

Dynamic cone beam computed tomography (CBCT) has been developed to provide respiratory phase correlated imaging in image guided therapy. The difficulty of acquisition of dynamic CBCT images is due to the fact that multiple phase binning of CBCT scans leading to insufficient number of projections available for image reconstruction. By making use of the redundant information shared by constituent scans, we proposed a computational model to reconstruct dynamic CBCT images with relatively high spatial resolution as well as utilizing the temporal coherence.

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MS120

Qualitative Assessment of the Role of Climate Change on Malaria Transmission Dynamics

A new model for assessing the impact of climate change on malaria transmission dynamics is developed. The disease-free periodic solution of the resulting non-autonomous deterministic model is shown to be locally-asymptotically stable when the associated basic reproduction ratio is less than unity. The disease persists in the community when the reproduction ratio is greater than unity. The effect of uncertainties of the estimates of the parameter values used in the numerical simulations of the model is analyzed. Numerical simulations of the model suggest that disease burden increases with increasing temperature (as measured in terms of the cumulative number of new cases and malaria-induced mortality) in the community. Furthermore, simulations of the autonomous version of the model suggest that personal protection measures (against mosquito bites) are marginally more effective than mosquito-reduction measures. As expected, the universal anti-malaria strategy (which combines both mosquito-reduction and personal protection strategies) is the most effective means to combat the spread of malaria in the population.

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MS120

A Structured Avian Influenza Model with Imperfect Vaccination

We introduce a model of avian influenza in domestic birds with imperfect vaccination and age-since-vaccination structure. The model has four components: susceptible birds, vaccinated birds (stratified by vaccination-age), asymptomatically infected birds, and infected birds. The model includes reduction of probability of infection, decreasing severity of disease of vaccinated birds and vaccine waning. The basic reproduction number, $\mathcal{R}_0$, is calculated. The disease-free equilibrium is found to be globally stable under certain conditions when $\mathcal{R}_0 < 1$. When $\mathcal{R}_0 > 1$, existence of an endemic equilibrium is proved (with uniqueness for the ODE case and local stability under stricter conditions) and uniform persistence of the disease is established. The inclusion of reduction in susceptibility of vaccinated birds, reduction in infectiousness of asymptomatically infected birds and vaccine waning can have important implications for disease control. We analytically and numerically demonstrate that vaccination can paradoxically increase the total number of infected, resulting in the "silent spread' of the disease. We also study the effects of vaccine efficacy on disease prevalence and the minimum critical vaccination coverage, a threshold value for vaccination coverage to avoid an increase in total disease prevalence due to asymptomatic infection.

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MS120

Modeling Avian Influenza and Implications for Control

A mathematical model of avian influenza which involves human influenza is introduced to better understand the complex epidemiology of avian influenza. The model is used to rank the efficacy of the current control measures. We find that culling without re-population and vaccination are the two most efficient control measures. Control measures applied to humans, such as wearing protective gear, are not very efficient. Furthermore, we find that should a pandemic strain emerge, it will invade, possibly displacing the human influenza virus in circulation at that time. Moreover, higher prevalence levels of human influenza will obstruct the invasion capabilities of the pandemic H5N1 strain. This effect is not very pronounced, as we find that 1% increase in human influenza prevalence will decrease the invasion capabilities of the pandemic strain with 0.006%.

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MS120

Evaluation of Malaria Vaccines as a Control Strategy in a Region with Naturally Acquired Immunity

The malaria vaccine RTS,S has reached the final stages of vaccine trials, demonstrating an efficacy of roughly 50% in children. Regions with high prevalence tend to have high levels of naturally acquired immunity (NAI) to severe malaria. I will introduce a model developed to address concerns about how these vaccines will perform in regions with existing NAI, discuss some analytic results and their public health implications, and reframe our question as an optimal control problem.

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MS121

Undergraduate Modeling Curricula

Abstract not available at time of publication.

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MS121

Modeling in the Early Grades

Abstract not available at time of publication.

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MS121

Mathematical Modeling in High School

Abstract not available at time of publication.

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MS121

SIAM-NSF Modeling across the Curriculum initiative and Workshops: Introduction

Abstract not available at time of publication.

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MS122

Reduced Order Modeling of the Quasi-Geostrophic Equations

This talk surveys some recent developments in the modeling, analysis and numerical simulation of the quasi-geostrophic equations, which describe the wind-driven large scale ocean circulation. A new large eddy simulation model, which is based on approximate deconvolution, is proposed for the numerical simulation of the one-layer and two-layer quasi-geostrophic equations. A reduced order model based on the proper orthogonal decomposition is also proposed as an accurate and computationally efficient tool for the numerical simulation of the quasi-geostrophic equations. The error analysis for the finite element discretization and the numerical investigation of the new models are also presented.

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MS122

Fluid-Structure Interaction Decoupling by Optimization

Simulating fluid-structure interactions is challenging due to the tight coupling between the fluid and solid substructures. An approach is presented that allows the problem to be decoupled by reformulating it in an optimal control setting. A control is introduced to minimize the jump in velocity and stress on the interface. An analytical framework is developed to show the well-posedness of the optimality system for the time dependent case.

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MS122

Numerical Approximation of Non-Newtonian Fluid - Structure Interaction Problems

Fluid-structure interaction (FSI) problems governed by non-Newtonian fluid models are considered. For viscoelastic and quasi-Newtonian fluid models variational formulations of the coupled FIS systems are developed based on the Arbitrary Lagrangian-Eulerian (ALE) method. Stability of the time discretized systems and finite element error estimates are discussed, and numerical results will be presented.

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MS122

Greenland Ice-sheet Initialization: Optimal Control and Bayesian Calibration Approaches

Greenland ice sheet plays a significant role in climatology and, in particular, in sea-level rise. In order to simulate the evolution of the ice sheets we need to know the current thermomechanical state of the system. In this talk, we seek an initial state for the Greenland ice sheet via the estimation of the basal sliding coefficient and the bedrock topography. We consider both a deterministic approach (PDE constrained optimization) and a Bayesian calibration approach.

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MS123

Optimal Shrinkage of Singular Values

It is common practice in multivariate statistical analysis to reduce dimensionality by performing SVD or PCA, and keeping only r singular values. For white noise and appropriate asymptotic frameworks, random matrix theory describes the random behavior of the singular values and vectors of Y. It delivers simple, convincing answers to a range of fundamental questions, such as the location of the optimal singular value threshold and the shape of the optimal singular value shrinker.

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MS123

Tensor GSVD for Comparison of Two Column-Matched and Row-Independent Large-Scale Biomedical Datasets

There exists a fundamental need for frameworks that can simultaneously compare and contrast large-scale data tensors, e.g., biomedical datasets recording multiple aspects of a disease across a set of patients. We describe a novel exact and unique simultaneous decomposition for two tensors that generalizes the GSVD to a tensor GSVD. We show that tensor GSVD comparisons of two ovarian cancer patient- and platform-matched genomic datasets from The Cancer Genome Atlas predict survival and drug targets.

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MS123

Pattern Discovery and Cancer Gene Identification in Integrated Cancer Genomic Data

We propose a latent variable approach for joint clustering of discrete and continuous variables that arise from integrated genomic, epigenomic, and transcriptomic profiling in large-scale genome characterization studies. A penalized likelihood approach is implemented for variable selection. We show application of the method to The Cancer Genome Atlas (TCGA) pan-cancer cohort with whole-exome DNA sequencing, SNP 6.0 array, and mRNA sequencing data in 3,000 patient samples spanning 12 cancer types.

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MS123

Breaking the Curse of Dimensionality Using Decompositions of Incomplete Tensors

The number of elements in higher-order tensors scales exponentially in the number of dimensions as do the computation and memory costs. Because of this, working with very large full tensors becomes infeasible. To alleviate or break this *curse of dimensionality*, tensor decompositions can be used instead. We discuss such decompositions and structure-exploiting, compressed sensing-type algorithms to compute these decompositions of large tensors while using only a small fraction of known elements.

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MS124

Div First-Order System LL* for Elliptic Systems

The first-order system LL* (FOSLL*) approach was introduced in order to retain the full efficiency of the L^2 norm first-order system least-squares (FOSLS) approach while exhibiting the generality of the inverse-norm FOSLS approach. In this talk, we will present the div FOSLL* approach to the Stokes and linear elasticity equations and the a priori and a posteriori error estimations.

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MS124

What Kinds of Singularities can we Deduce from the Corner Singularity Theory of the Compressible Viscous Stokes Flows?

Based on some known corner singularity and regularity results for the compressible viscous Stokes equations, I will describe certain singularities of solutions in the domain, for instance, interior layer, jump discontinuities of the density solution across the streamline emanating from the nonconvex vertex or grazing vertex.

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MS124

Compact Implicit Integration Factor Method for High Order Differential Equations

When developing efficient numerical methods for solving parabolic types of equations, severe temporal stability constraints on the time step are often required due to the high-order spatial derivatives and/or stiff reactions. The implicit integration factor (IIF) method, which treats spatial derivative terms explicitly and reaction terms implicitly, can provide excellent stability properties in time with nice accuracy. One major challenge for the IIF is the storage and calculation of the dense exponentials of the sparse discretization matrices resulted from the linear differential operators. The compact representation of the IIF (cIIF) can overcome this shortcoming and greatly save computational cost and storage. On the other hand, the cIIF is often hard to be directly applied to deal with problems involving cross derivatives. In this talk, by treating the discretization matrices in diagonalized forms, we present an efficient cIIF method for solving a family of semilinear fourth-order parabolic equations, in which the bi-Laplace operator is explicitly handled and the computational cost and storage remain the same as to the classic cIIF for second-order problems. In particular, the proposed method can deal with not only stiff nonlinear reaction terms but also various types of homogeneous or inhomogeneous boundary conditions. Numerical experiments are finally presented to demonstrate effectiveness and accuracy of the proposed method.

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MS124

An Asymptotic Splitting Approximation for Highly Accurate Numerical Solutions of Differential Equations

This talk explores applications of the asymptotic splitting method for approximating highly oscillatory solutions of the systems of paraxial Helmholtz equations. An eikonal transformation is introduced for oscillation-free platforms and matrix operator decompositions. It is found that the sequential, parallel and combined exponential splitting formulas possess not only anticipated algorithmic simplicity and efficiency, but also the accuracy and asymptotic stability required for highly oscillatory wave computations via systems of partial differential equations.

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MS125

Recent Progress in MatCont Development

MatCont is an interactive MATLAB software for numerical analysis of ODEs in $\mathbf{R}^n$. It allows to simulate ODEs, continue equlibria and cycles in one parameter, and study bifurcations of equilibria, cycles, and homoclinic orbits in two-parameter ODEs. Recent features of MatCont will be presented, including normal form computations for codim 2 bifurcations of cycles and initialization of homoclinic orbits. Decisions made during the development and future of the software will be discussed.

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MS125

Numerical Analysis of Travelling Waves in Neural Fields

We consider waves in integro-differential systems modelling neural activity. For special cases of spatial coupling a suitable ODE can be derived whose solutions correspond to patterns of the original system. We exploit the numerical toolbox MATCONT to construct a complete bifurcation diagram for smooth nonlinearities. For more general, but translationally invariant connectivity including transmission delays, we propose novel numerical schemes to compute travelling waves and discuss its implementation.

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MS125

(Parallel) Auto and Applications: Past, Present and Future

We show how the numerical continuation package AUTO-07p can effectively run in parallel using MPI on modern HPC clusters, and explain its algorithms. Much larger problems can now be continued than was reasonably possible in the past. Combining with the method of continuation of orbit segments we can investigate how certain ODE and PDE solutions suddenly change as parameters cross critical values. Several examples illustrate this technique. Lastly, possible future directions for AUTO are given.

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MS125

Analysis of Nonsmooth Systems: Perspectives and Directions

The realisation that many real-world systems possess nonsmooth characteristics has opened up a plethora of different directions for the analysis of such systems. In this presentation I will give a background to nonsmooth systems, describe a few of the analysis techniques employed, and also discuss where the field is heading. Open problems that will keep the dynamical systems community busy for years to come will be highlighted through a couple of examples.

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MS126

A Locally Accelerated Block Preconditioned Steepest Descent Method for Ill-conditioned Generalized Hermitian Eigenvalue Problems

In this talk, we first present a locally accelerated block preconditioned steepest descent (LABPSD) algorithm for solving ill-conditioned generalized Hermitian eigenvalue problems, such as arising in orbital based *ab initio* methods for electronic structure calculations. We then revisit the classical convergence analysis of steepest descent algorithms and provide a new analysis to justify the efficiency of LABPSD.

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MS126

Structured Eigensolvers for the Analysis of Symmetry-Breaking in Next Generation Gyroscopes

In 1890, G. H. Bryan demonstrated that when a ringing wine glass rotates, the shape of the vibration pattern precesses. This effect is the basis for a family of high-precision gyroscopes. Mathematically, the precession can be described in terms of a symmetry-breaking perturbation due to gyroscopic effects of a geometrically degenerate pair of vibration modes. Unfortunately, current attempts to miniaturize these gyroscope designs are subject to fabrication imperfections that also break the device symmetry. In this talk, we describe the structure of the eigenvalue problems that arise in simulation of both ideal and imperfect geometries, and show how to use this structure in accurate and efficient simulations.

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MS126

Fast Spectral Computations for Quasiperiodic Schroedinger Operators

Discrete Schrödinger operators with quasiperiodic potentials arise as mathematical models of quasicrystals. Their spectra exhibit exotic properties that are more challenging to analyze than periodic or random potentials; often these spectra are Cantor sets. Quasiperiodic potentials can be approximated by periodic potentials, whose spectrum can be computed by solving finite dimensional eigenvalue problems. Accurate estimates require long periods. We show how to compute such approximations quickly and address the need for high accuracy.

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MS126

Eigenvalue Problems in Electron Excitation

Single-electron excitation can be described by a nonlinear eigenvalue known as Dyson's equation in which the Hamiltonian operator is a function of an eigenvalue to be determined. We will describe the nonlinear structure of the eigenvalue problem and examine numerical methods for solving this type of problem.

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MS127

Rheology of Sickle Cell Anemia: Effects of Heterogeneous RBC Shapes

Sickle cell anemia (SCA) is a a highly complex, inherited blood disorder exhibiting heterogeneous cell morphology and abnormal rheology. To better understand the relationship between rheological behavior and cell morphological characteristics of blood in SCA, we present a multi-scale sickle red blood cell (SS-RBC) model, accounting for diversity in both cell shape and rigidity. The proposed model provides a systematical approach to quantify the rheological behavior and hemodynamics of SS-RBC suspensions. We quantify the heterogeneous shear viscosity of SS-RBC suspensions with different cell morphologies, *i.e.*, the SS-RBC suspensions with granular shapes are the most viscous; while the shear viscosity of SS-RBC suspensions containing elongated cells show a dramatic decrease. In combination with the experimental data of SS-RBCs from patients treated with and without hydroxyurea, we also predict the shear viscosity of SS-RBC suspensions under different conditions. These findings lead to useful insights into the abnormal rheological behavior of blood in SCA.

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MS127

Lipid Bilayer and Cytoskeletal Interactions in a Red Blood Cell

We developed a two-component model of red blood cell (RBC) membranes to study interactions between the lipid bilayer and the cytoskeleton for healthy and diseased RBCs. We modeled the bilayer and the cytoskeleton as two distinct components and consider the normal elastic interaction and tangential viscous friction between them. We implemented this model using both a three-level multiscale continuum approach and Dissipative Particle Dynamics, and investigated RBC-related diseases such as malaria and sickle cell disease.

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MS127

Three-Dimensional Vesicle Electrohydrodynamics: A Level Set Method

The electrohydrodynamics of three-dimensional vesicles is investigated using a combined Jet level set/continuum force method. The electric field in the domain is obtained by an immersed interface method, for which the necessary jump conditions have been developed. Numerical results match well with the dynamics observed experimentally. A investigation of parameters influencing the vesicles dynamics will also be presented.

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MS127

A Hybrid Numerical Method for Electro-Kinetic Flow with Deformable Membranes

We consider two-phase flow of ionic fluids whose motion is driven by an imposed electric field. At a fluid-fluid interface, a screening cloud of ions develops and forms an electro-chemical double layer or 'Debye layer'. The applied electric field acts on the ionic cloud it induces, resulting in a strong slip flow near the interface. This is known as 'induced-charge electro-kinetic flow', and is an important phenomenon in microfluidic applications and in the manipulation of biological cells. We address a significant challenge in the numerical computation of such flows in the thin-double-layer limit, by using the slenderness of the layer to develop a fast and accurate 'hybrid' or multiscale numerical method. The method incorporates an asymptotic analysis of the electric potential and fluid dynamics in the Debye layer into a boundary integral numerical solution of the full moving boundary problem.

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MS128

Integral Equations on Domains with Edges

We will discuss the discretization of integral equations on surfaces with edges and corner points. Although achieving high accuracy in this setting is not that difficult, there are a number of issues (such as the need for highly anisotropic meshes) which make the construction of efficient discretization procedures challenging. We will discuss our progress on addressing these issues.

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MS128

Integral Equation Techniques for Solving Elliptic Problems with Mixed Boundary Conditions

This talk describes integral equation techniques for solving elliptic problems with mixed boundary conditions (i.e. a portion of the obstacle has Dirichlet boundary conditions while the remainder has Neumann boundary conditions.) The proposed approach avoids using a hypersingular kernel as a result the system is better conditioned than existing integral equation based methods. For many problems, the discretized system is amenable linear scaling solvers. Numerical experiments illustrate the performance of the solution technique.

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MS128

Practical and Efficient Direct Solvers for BIEs

The last several years have seen rapid progress on constructing direct solvers for the dense linear systems arising upon discretization of BIEs. The goal is to build direct solvers with $O(N^p)$ complexity, where p is one, or close to one, and with high practical efficiency. This talk will describe techniques aimed at improving performance and simplifying coding by using randomized methods to accelerate certain structured matrix computations.

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MS128

Updating Techniques for Hierarchical Factorizations

Many fast direct algorithms for solving linear systems arising from discretized partial differential equations or boundary integral equations rely on a hierarchical tree decomposition of the domain, e.g., methods based on nested dissection for PDEs or recursive skeletonization for integral equations. In this talk we will show that, given a factorization corresponding to a given problem, we can update the factorization to solve problems related by local changes such as localized modification of the PDE coefficients or perturbation of the problem geometry. In cases where the computational cost per tree node is the same across all nodes, updating is both asymptotically and practically less expensive than re-doing the complete factorization.

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MS129

Diffusion-Limited Growth and Decay of 2D Epitaxial Nanoclusters: Atomistic and Coarse-Grained Modeling

Random deposition onto isotropic or anisotropic crystalline surfaces leads to diffusion-mediated formation of an ensemble of epitaxial 2D islands or nanoclusters. The process might be described by stochastic fully atomistic-level models or by coarse-grained 2D continuum descriptions of surface diffusion and aggregation. However, the latter must retain the stochastic aspects of nucleation, and an open challenge is to capture far-from equilibrium island growth shapes (as this requires precise treatment of non-equilibrium diffusion around island edges). After deposition, these island ensembles coarsen usually by Ostwald ripening. Again atomistic or continuum-level treatment is possible, the latter being more common. However, recent experiments reveal shortcomings of standard continuum formulations for strongly anisotropic systems, a feature which we address.

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MS129

Efficient Numerical Methods for Molecular Beam Epitaxial Growth

This work is concerned with efficient numerical methods for the simulation of the dynamics of molecular beam epitaxial (MBE) growth. Numerical simulations of MBE models require long time computations, and therefore large time-stepping methods become necessary. In this work, we present some unconditionally energy stable finite difference schemes for MBE models. We will also discuss on some time adaptive strategies.

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MS129

Stable and Convergent Numerical Schemes for Phase Field Crystal Models

Crystalline materials have atomic-scale imperfections in the form of defects – such as vacancies, grain boundaries, and dislocations – and controlling, or at least predicting, the formation and evolution of such imperfections is a major challenge. The phase field crystal (PFC) methodology has emerged as a important, increasingly-preferred modeling framework for investigating materials with atomic-scale structures on diffusive time scales. In essence, the fast atomic vibrational time-scale phenomena are averaged out, but the atomic spatial resolution is preserved. In this talk, I describe some efficient, stable, and convergent numerical methods for some PFC and PFC-type equations, a family of highly nonlinear hyperbolic-parabolic PDE and integro-PDE. I will also discuss a new PFC framework for multi-spatial-scale modeling based on the recent method of amplitude expansions.

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MS129

Continuum Framework for Dislocation Structure, Energy and Dynamics of Dislocation Arrays and Low Angle Grain Boundaries

We present a continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. In our continuum framework, we define a dislocation density potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocation in a very simple and accurate way. The continuum formulations of energy and dynamics include the long-range interaction of constituent dislocations, local line tension effect of dislocations and the cooperative motion of dislocations, which are derived from the discrete dislocation model. We also present numerical simulations using this continuum model including applications to dislocation structures of low angle grain boundaries and interfaces with misfitting spherical inclusions.

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MS130

An Adaptive RBF-WENO Method for Hyperbolic Problems

An adaptive RBF-WENO method is proposed. The RBF-WENO hybrid method is to use the radial basis function interpolation replacing the polynomial interpolation. We show that the locally adapted shape parameters can elevate the regular WENO order resulting better accuracy and convergence. Numerical examples are provided.

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MS130

Matrix-Valued Kernels Associated to Vector-

Valued Random Fields with Correlated Components

We propose a class of nonseparable space-time compactly supported correlation functions, termed here quasi-tapers, to mean that such correlations can be dynamically compactly supported over space or time. An important feature of the quasi-taper is given by a spatial (temporal) compact support being a decreasing function of the temporal lag (spatial distance), so that the spatial (temporal) compact support becomes smaller when the temporal (spatial) dependence becomes weaker. We propose general classes as well as some examples that generalize the Wendland tapers to the space-time setting. Then a non separable space-time taper with spatial and temporal compact support is obtained as tensor product of quasi-tapers. Our space-time taper includes all the known constructions as special cases and will be shown to have great exibility. Covariance tapering is then explored as an alternative to maximum likelihood when estimating the covariance model of a space-time Gaussian random field in the case of large datasets. The proposed quasi and space-time tapers allows to perform covariance tapering when dealing with data that are densely observed in time (space) but sparse in space (time) or densely observed both in time and space. The statistical and computational properties of the space-time covariance tapering is addressed under increasing domain asymptotics. A simulation study and two real data examples illustrate the statistical and computational performances of the covariance tapering with respect to the maximum likelihood method using the space-time tapers proposed.

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MS130

Improved Exponential Convergence Rates for Regularized Approximation by Oversampling Near the Boundary

We discuss convergence rates for kernel based approximation in smooth settings. Typical examples range from classical function approximation to the approximate solution of partial differential equations. In smooth settings one expects exponential convergence orders, but the numerical schemes are notoriously ill conditioned, which enforces some kind of regularization. Further, in smooth settings one often observes boundary effects, i.e., the deterministic approximation rates for scattered data approximation are improved globally if the data sets are distributed more densely near the boundary. In this talk, such boundary effects for regularized approximation schemes are analyzed by means of sampling inequalities for smooth functions. The latter provide a bound on a continuous norm in terms of a discrete norm and an error term that tends to zero exponentially as the discrete data set becomes dense. We show that the exponential convergence rates are improved by oversampling near the boundary.
This is partly based on joint works with Christian Rieger (Bonn) and Robert Schaback (Göttingen).

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MS130

Recurrence Operators for Zonal Basis Functions on the Sphere

One approach for simulation of stationary random fields in the Euclidean space is based on Matheron's turning bands methods. The idea behind this method is to relate positive definite radial functions in the $\mathbb{R}^d$ to corresponing ones on the circle using averaging. The explicit form of the turning bands operator turns out to be a special case of a well-known recurrence relation for Bessel functions. Aiming at similar recurrences for zonal basis functions on the sphere, we can use relations between Gegenbauer polynomials of different parameters. Interestingly, there is a set of operators which can be used to derive analogous relations. We will discuss some of these operators and their interrelations.

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MS131

Tracking a Low-Dimensional Vector Via Quantized Measurements Or Pairwise Comparisons

Suppose that we wish to track a point $x_t \in \mathbb{R}^k$ as its position changes in time. In this talk I will describe approaches to this problem in two practical settings. First, I will consider the case where the observations consist of highly quantized linear measurements. Next I will describe the related case where our data is given by pairwise comparisons between between x_t and various points $x_1, \ldots, x_n \in \mathbb{R}^k$ with known position. I will describe practical algorithms for handling both cases.

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MS131

Intrinsic Volumes of Convex Cones: Theory and Applications

Spherical intrinsic volumes are fundamental statistics of convex cones, and occupy a central role in integral geometry. They also appear in various guises in statistics, convex optimization, compressed sensing (polytope angles), algebraic combinatorics, and differential geometry, among other fields. In particular, they are the main ingredients of the classical kinematic formulas, which describe the exact intersection probabilities of randomly oriented cones. Combining the kinematic formula with another pillar of integral geometry, the spherical Steiner formula, and concentration of measure arguments, gives rise to a complete explanation of phase transition phenomena for general random convex optimization problems. This talk surveys the theory of intrinsic volumes, present methods of computation, and highlights connections to problems in statistics, convex regularization, and to the theory of condition numbers for convex optimization. Based on joint work with Dennis Amelunxen, Mike McCoy and Joel Tropp

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MS131

The Achievable Performance of Demixing

Demixing is the problem of disentangling multiple informative signals from a single observation. These problems appear frequently in image processing, wireless communications, machine learning, statistics, and other data-intensive fields. Convex optimization provides a powerful framework for creating tractable demixing procedures that work right out of the box. In this talk, we describe a geometric theory that precisely characterizes the performance of convex demixing methods under a generic model. This theory precisely identifies when demixing can succeed, and when it cannot, and further indicates that a sharp phase transition between success and failure is a ubiquitous feature of these programs. Our results admit an elegant interpretation: Each signal has an intrinsic dimensionality, and demixing can succeed if (and only if) the number of measurements exceeds the total dimensionality in the signal. Joint work with Joel A. Tropp.

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MS131

Adaptively Sensing in Compressive Sensing Applications

In this talk we will present new results in compressive sensing using adaptive sampling. Compressive sensing is a new signal acquisition technology which reconstructs a high dimensional signal from a small number of linear measurements. In the typical setting, these measurements are determined a priori. However, in some cases selecting these measurements adaptively can lead to improvements both in error and in the number of samples required. We discuss some fundamental limitations of this sampling scheme, as well as some new encouraging results which show compressive sensing can benefit from adaptivity.

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MS132

Building Meso-Scale Stochastic Models Using the Mori-Zwanzig Formalism

We present a meso-scale model built from the Mori-Zwanzig (MZ) formalism. The meso-scale model is built with the projection operator that is applied on the discretized MZ equation in time. The projection operator is used to calculate the memory function with a simple recurrence without having to compute orthogonal dynamics, or e^{sQL}. Assuming that the memory function can be well-approximated by exponentials, we can generate the corresponding fluctuation using Ornstein-Ulenbeck process. Then we can obtain the generalized Langevin equation. Our approach was validated by the simple heat bath model, in which the analytical solution is known. The Dissipative Particle Dynamics (DPD) system with one tagged particle was also used as a numerical test case. Finally, we apply our framework to generate the meso-scale model of alanine dipeptide (in Φ and Ψ dihedral angle) to correctly predict kinetics of the bio-molecule.

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MS132

The Reduction of Molecular Dynamics Models Using Mori-Zwanzig Projection Formalism

Molecular dynamics models find applications in many areas of applied sciences. One often needs to restrict the simulations to localized regions to minimize the computational cost. I will present the Mori-Zwanzig formalism as a systematic approach to coarse-grain molecular dynamics models. In particular, I will discuss how to approximate the memory functions, and how to sample random noises. As example, simulations of crack propagation, dislocation dynamics, and protein dynamics will be presented.

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MS132

Stochastic Modeling Through the Mori-Zwanzig Formalism

The Mori-Zwanzig formalism tells us that if we project a dynamical system onto a subset of its degrees of freedom, the resulting process will generally exhibit memory effects. Unfortunately, the associated memory kernels, which are needed for dimension reduction, are typically difficult to obtain directly from the formalism itself. In this talk, we propose an empirical approach based on statistical estimation and apply it to certain prototypical models of spatiotemporal chaos.

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MS132

MZ-PDF Methods for Stochastic Analysis in Nonlinear Dynamical Systems

We propose a new framework for stochastic analysis in nonlinear dynamical systems based on goal-oriented probability density function (PDF) methods. The key idea stems from techniques of irreversible statistical mechanics, and it relies on deriving reduced-order PDF equations for quantities of interest, e.g., functionals of the solution to systems of stochastic ordinary and partial differential equations. The proposed approach is useful to many disciplines as it leads to new and more efficient computational algorithms.

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MS133

A Predator-prey-disease Model with Immune Response in Infected-prey

This talk presents a predator-prey-disease model with immune response in the infected prey. The basic reproduction number of the within-host model will be defined and it is found that there are three equilibria: extinction equilibrium, infection-free equilibrium and infection-persistent equilibrium. The stabilities of these equilibria are completely determined by the reproduction number of the within-host model. Furthermore, a basic reproduction number of the between-host model and two predator invasion numbers exists along with a predator invasion number in the absence of disease and predator invasion number in the presence of disease. There also exists a predator and infection-free equilibrium, infection-free equilibrium, predator-free equilibrium and a coexistence equilibrium. The local stabilities of these equilibria under certain conditions depending on the basic reproduction and invasion reproduction numbers shall be explained in this talk. Finally the global stability of the predator-free equilibrium will be explained in this talk.

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MS133

Modeling the Spread of Bacterial Infections in a Hospital with Environmental Contamination

Nosocomial infections, i.e. hospital-acquired infections, have become a major concern for public health officials as the amount of antibiotic-resistant bacterial infections increases. One important mechanism for bacterial persistence is the ability of bacteria to contaminate hospital surfaces and survive in this environment for extended periods of time. In this talk, I discuss a differential equation model of bacterial infections in a hospital with environmental contamination. The basic reproduction number of the model is proved to be a global threshold under certain conditions. In addition, simulations of the deterministic model and a stochastic version of the model provide insight into an outbreak of bacterial infections in a hospital. This is joint work with Glenn Webb.

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MS133

Model of Spontaneous HIV Infection Control Following Cessation of Antiretroviral Therapy

Reports suggest that HIV antiretroviral therapy initiated early may permit post-treatment control (PTC) of HIV (undetectable viral load) after treatment termination. We hypothesize that early treatment induces PTC by restricting the latent reservoir size, allowing immune responses to control infection post-treatment. ODE model analysis reveals a range in immune response-strengths where a patient may show viral rebound or PTC. In this bistable regime, we predict a latent reservoir size threshold below which PTC is achievable.

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MS133

Dyanamics of Low and High Pathogenic Avian Influenza in Wild and Domestic Bird Populations

An earlier infection with low pathogenic avian influenza (LPAI) provides a partial immunity towards infection with high pathogenic avian influenza (HPAI). We consider a time-since recovery structured model to study the dynamics of LPAI and HPAI in wild and domestic bird populations. The system has a unique disease-free equilibrium which is locally and globally stable when the reproduction number is less than one. There are unique LPAI-only and HPAI-only equlibria, which are locally asymptotically stable as long as the other pathogen can not invade the equilibrium. There exist a coexistence equilibirum when the invasion number of both pathogens are greater than one. We show that both pathogen can coexist in the form of sustained oscillations.

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MS134

Inverting for Maritime Environments Using Empirical Eigenfunction Bases from Radar Imagery

Radar wave front arrival times and spatial energy deposition, associated with propagation through a given marine atmospheric boundary layer, may be described using proper orthogonal modes, and subsequently represented as points on the compact Stiefel manifold. By exploiting the Riemannian structure of Stiefel, interpolation within the cloud of manifold points is possible when solving inverse problems aimed at uncovering *in situ* maritime conditions affecting radar propagation on a given day.

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MS134

Optimal Filters for General-Form Tikhonov Regularization

In this work, we use training data in an empirical Bayes risk framework to estimate optimal regularization parameters for the general-form Tikhonov problem and the multi-parameter Tikhonov problem. We will show how estimates of the optimal regularization parameters can be efficiently obtained and present several numerical examples from signal and image deconvolution to demonstrate their performance.

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MS134

Reproducible Kernel Hilbert Space Modeling and Computing in Imaging

Regularization ensures uniqueness and smoothness in various inverse problems arisen in imaging science. Most of the existing regularization methods can not efficiently interpolate or extrapolate image intensity. They are thus not effective in solving image super-resolution and inpainting problems that both need to extend intensity information at one region to another. We use reproducible kernel Hilbert space (RKHS) to model these two problems. RKHS method is more flexible, adaptive to data and involves simple computation.

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MS134

Improved Image Reconstruction by Statistically Estimating Near-Optimal Parameters for Spectral Filters

Spectral Filters improve the reconstruction of images corrupted by blur and unknown noise. We compute in this work the near-optimal parameters for general filters such as a hybrid method that combines the Tikhonov filter and the truncated SVD. Using the discrete Picard condition, we provide an algorithm for computing a Picard parameter, a cut-off for the singular values beyond which the observations are predominantly noise. The method compares favorably against other reconstruction methods.

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MS135

Considerations in the Design of Numerical Schemes for Geophysical Flows

Long-term simulations of geophysical flows, e.g. in predicting the climate change for the next century, require numerical schemes that conserve key quantities and accurately represent internal wave propagations, all at reasonable computational costs. In this talk, we will briefly review the classical staggering-grid techniques proposed by Arakawa et al almost forty years ago. Some recent developments will be presented, and ideas for future work will also be discussed.

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MS135

Finite Volume Approximation of the Inviscid Primitive Equations in a Complex Domain

We construct the cell-centered Finite Volume discretization of the two-dimensional inviscid primitive equations in a domain with topography. To compute the numerical fluxes, the so-called Upwind Scheme (US) and the Central-Upwind Scheme (CUS) are introduced. We verify, with our numerical simulations, that the US (or CUS) is a robust first (or second) order scheme, regardless of the shape or size of the topography and without any mesh refinement near the topography.

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MS135

Approximation of the Singularly Perturbed Equations of Parabolic Type in a Circular Domain

In this talk, I will present convergence results of singularly perturbed problems in a circular domain and provide as well approximation schemes, error estimates and numerical simulations. To resolve the oscillations of classical numerical solutions due to the stiffness of our problem, we construct, via boundary layer analysis, the so-called boundary layer elements which absorb the boundary layer singularities. Using a P1 classical finite element space enriched with the boundary layer elements, we obtain an accurate numerical scheme in a quasi-uniform mesh.

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MS135

POD Reduced-order Models of Complex Fluid Flows

The proper orthogonal decomposition (POD) method has been commonly applied to generate reduced-order models for turbulent flows. However, to achieve a balance between the low computational cost required by a reduced-order model and the complexity of the targeted turbulent flows, appropriate closure modeling strategies are needed. In this talk, we present several new nonlinear closure methods for the POD reduced-order models, which synthesize ideas originating from large eddy simulation. We design efficient discretization algorithms for the new models and perform the numerical validation and verification in challenging computational settings.

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MS136

Distribution of Directional Change as a Signature of Complex Dynamics

Analyses of random walks traditionally use the mean square displacement (MSD) as an order parameter characterizing dynamics. We show that the distribution of relative angles of motion between successive time intervals of random walks in two or more dimensions provides information about stochastic processes beyond the MSD. We illustrate the behavior of this measure for common models and apply it to experimental particle tracking data. For a colloidal system, the distribution of relative angles reports sensitively on caging as the density varies. For transport mediated by molecular motors on filament networks in vitro and in vivo, we discover self-similar properties that cannot be described by existing models and discuss possible scenarios that can lead to the elucidated statistical features.

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MS136

Honeybee Nest Bentilation: A Bio-robotic Study of Collective Flapping Wing Fluid Mechanics

Honeybee workers ventilate their hive by collectively fanning their wings. The fluid mechanics of this phenomena—in which wings continuously operate in unsteady oncoming flows (i.e. the wake of neighboring worker bees) and near the ground—are unstudied and may play an important role in the physiology of colony life. We perform field and laboratory observations of nest ventilation wing kinematics. Through recent advances in micro-robotics we construct at scale micro-mechanical models of honeybee ventilation swarms to explore the fluid mechanics of collective ventilation.

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MS136

Propagating Waves Structure Spatiotemporal Activity in Visual Cortex of the Awake Monkey

Propagating waves have recently been found in the neocortex of anesthetized animals. Whether propagating waves appear during awake and conscious states, however, remains unclear. To address this, we apply a phase-based analysis to single-trial voltage-sensitive dye imaging data, which captures the average membrane potential of neuronal populations over large cortical areas with high spatiotemporal resolution. With this approach, we detect and characterize spontaneous and stimulus-evoked propagating waves in visual cortex of the awake monkey.

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MS137

A Novel Higher Order ETD Scheme for System of Coupled Semi-linear PDEs

We introduce a novel version of the ETD3RK scheme based on $(1,2)-$Padé approximation to exponential function. In addition, we develop its extrapolation form to improve temporal accuracy to the fourth order. The scheme and its extrapolation are seen to be strongly stable and have ability to damp spurious oscillations. We demonstrate the performance of the schemes on system of nonlinear Schrödinger equations and problem from biochemistry which contains discontinuity between initial and boundary condition.

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MS137

Local Discontinuous Galerkin Method with a Fourth Order Exponential Time Differencing Scheme for System of Nonlinear Schrodinger Equations

This paper studies a local discontinuous Galerkin (LDG) approximation combined with fourth order exponential time differencing Runge-Kutta (ETDRK4) method for solving the N-coupled nonlinear Schrödinger equation (NLSE). The numerical method is proven to be highly efficient and stable for long-range soliton computations. Numerical examples with periodic boundary conditions are provided to illustrate the accuracy, efficiency and reliability of the proposed method.

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MS137

A New Family of Discontinuous Galerkin Methods for Linear and Nonlinear Partial Differential Equations

In this talk, we discuss a discontinuous Galerkin (DG) finite element differential calculus theory for approximating weak derivatives of Sobolev functions and piecewise Sobolev functions. By introducing numerical one-sided derivatives as building blocks, various first and second order numerical operators such as the gradient, divergence, Hessian, and Laplacian operator are defined, and their corresponding calculus rules are established. We show that several existing DG methods can be rewritten compactly using the proposed DG framework, and that new DG methods for linear and nonlinear PDEs are also obtained.

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MS137

Application of the Laplace Transform Method to Solving Evolution Problems

We are interested in the highest-possible order time discretization for solving parabolic problems. Recently the method of Laplace transform has been drawing an increasing attention. Instead of solving parabolic problems using time-marching algorithms, we attempt to solve the Laplace-transformed complex-valued elliptic equations in parallel. The inverse Laplace transform then gives the time-domain solutions by using exponentional convergent quadrature rules on carefully-chosen contours. We will give a short review on this approach and generalize the method to solving parabolic equations with time-dependent coefficients. The method will be shown to converge exponentially under suitable assumptions. We will discuss a couple of directions to generalize this approach.

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MS138

Uncover Deep Learning: Assess Online Learners Cognitive Presence in Mooc

The study will investigate learners cognitive presence level in a five-week MOOC data science course. Transcript analysis, social network analysis, learning records (i.e. frequency of views, grades), survey of perceived learning and satisfaction will be used to assess the learning process and outcomes. The results will reveal the levels of cognitive presence exhibited by learners, how their cognitive presence evolves overtime, and how their levels of cognitive presence correlate with their online behaviors and satisfactions.

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MS138

Coalition for Undergraduate Computational Science and Engineering Education - Proof of Concept

This talk will present the project funded by NSF TUES to create a cluster of collaborating institutions that combine students into common classes and use cyberlearning technologies to deliver and manage instruction. As an idea of scale-up project, we will discuss how to advance Undergraduate Computational Science Education through learning analytics, deep learning assessment and massive open online courses.

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MS138

Undergraduate Exploration of Agent-Based Modeling

The final week of a modeling and simulation course in fall, 2013, students explored agent-based models (ABMs) with NetLogo. Initially, they completed tutorials to develop models on unconstrained growth and average distance covered by random walkers. Besides revealing their utility, these models provided an opportunity to compare agent-based modeling with previously considered techniquessystem dynamics modeling, empirical modeling, and cellular automaton simulations. Improved test scores and positive questionnaire results support the success of this approach.

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MS138

The Ingenious Project and Other Initiatives

This talk will focus on aspects of the INGenIOuS Mathematical Sciences Workforce Development project that relate especially to computational applied mathematics education. The NSF-funded project was a joint venture of all the main professional societies (ASA, AMS, MAA and SIAM). The focus on workforce development led to a strong role for applied mathematical science education. This theme continues for the upcoming CBMS forum, which will focus on the first two years of college education.

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MS139

Mathematical Modeling and Discretization for Exascale Simulation

In simulations, the choices of mathematical models and their discretization significantly influence the properties of the resulting discrete systems. The advent of exascale computing is an opportunity to re-think the formulation and implementation of mathematical models and discretizations in ways that are more favorable for numerical integration on exascale machines. We will survey several promising research topics and the fundamental constraints involved in the process of expressing physical phenomena as fully discrete models.

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MS139

Resilient Algorithms and Computing Models

Abstract not available at time of publication.

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MS139

Discrete Solvers at the Exascale

Discrete solvers are crucial in scientific simulations. Moving to the exascale will put heavier demands on these kernels due to the need for increasing amounts of data locality and to obtain much higher factors of fine-grained parallelism. Thus, parallel solvers must adapt to this environment, and new algorithms and implementations must be developed to capitalize on the capabilities of future hardware. We will discuss several key topics that are potentially relevant in the exacale era.

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MS139

Hierarchical Multilevel Methods for Exascale Uncertainty Quantification and Optimization

The sustained increase in computational capabilities will enable new possibilities at the intersection of optimization and uncertainty quantification (UQ), including model calibration, robust control and design under uncertainty. However, numerous changes in scientific computing at extreme scales are expected to challenge the current UQ/optimization paradigm, wherein theses techniques are typically wrapped around a black-box simulation. This talk will focus on several multi-fidelity, hierarchical approximations for UQ/optimization that exploit greater levels of parallelism provided by emerging many-core architectures.

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MS140

The Behavior of a Quasi-Circular Vesicle During Drying Processes

A proposed method for the preservation of biological cells is through desiccation. We consider a two-dimensional, quasi-circular vesicle, whose boundary is an inextensible bilipid membrane wall but whose enclosed area varies owing to the osmotic transport of water through the membrane. The evolution of the vesicle's shape is computed and the effects of advection, diffusion and the membrane's permeability are analyzed and compared with conclusions drawn from recent level-set simulations.

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MS140

Electrohydrodynamics of Lipid Bilayer Vesicles in AC and DC Fields

Vesicles are closed, fluid-filled lipid bilayers which exhibit shape transitions in the presence of electric fields. Here we model the vesicle membrane as an infinitely thin, capacitive, area-incompressible interface with the surrounding fluids acting as charge-advecting leaky dielectrics, then use the boundary integral method to numerically investigate the dynamics of a vesicle in various electric field profiles. Finally, we present a comparison of our numerical results with recent small deformation theory and experimental data.

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MS140

Field Theoretic Approaches for Non-Spontaneous Deformation of Bilayers under Surface Director Energies

The shapes of membranes are continually changing in their aqueous environment. Often, these shape changes involve proteins but the mechanistic coupling between proteins and bilayers is poorly understood. In this talk, we will discuss some classical and field theoretic calculations which have given insight into membrane shape changes away from equilibrium and allowed us to evaluate a path of deformations leading to a least energy barrier between quasi-static membrane configurations.

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MS140

Deformation and Stability of Vesicles in Dc Electric Pulses

Electrohydrodynamics of vesicles are investigated under strong DC pulses. In an applied field, the membrane acts as a capacitor and the vesicle deforms into an oblate or prolate ellipsoid. If poration occurs, the membrane capacitor becomes short-circuited and leads to non-ellipsoidal shape and vesicle collapse. The evolution of vesicle shape is studied for DC pulses of different strength and duration. Membrane composition is varied to observe the effect of membrane viscosity, capacitance, and poration threshold.

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MS142

Fast Iterative Methods for The Variable Diffusion Coefficient Equation in a Disk

Variable coefficient diffusion equation has widespread applications in many areas of Physics, Engineering and Industrial research like the flow in porous media, tomography in image processing to mention a few. We present here fast, efficient iterative methods to solve this equation in a disk with applications to the Ginzburg Landau equation. Our technique is based on the solution of the Poisson equation in a disk using fast Fourier transform and recursive relations. The method takes advantage of scaling the original problem and using shifted iteration. This is an ongoing work and our focus is to develop a fast solution for this non-seperable elliptic equation in arbitrary two-dimensional domains by the help of domain embedding method using the optimal distributed control algorithm. The performance of this fast method is illustrated with some numerical examples.

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MS142

Subspace Iteration Randomization and Low-rank Approximation

A classical problem in matrix computations is the efficient and reliable approximation of a given matrix by a matrix of lower rank. The truncated singular value decomposition (SVD) is known to provide the best such approximation for any given fixed rank. However, the SVD is also known to be very costly to compute. Among the different approaches in the literature for computing low-rank approximations, randomized algorithms have attracted researchers' recent attention due to their surprising reliability and computational efficiency in different application areas. Typically, such algorithms are shown to compute with very high probability low-rank approximations that are within a constant factor from optimal, and are known to perform even better in many practical situations. In this paper, we present a novel error analysis that considers randomized algorithms within the subspace iteration framework and show with very high probability that highly accurate low-rank approximations as well as singular values can indeed be computed quickly for matrices with rapidly decaying singular values. Furthermore, we show that the low-rank approximations computed by these randomized algorithms are actually rank-revealing approximations, and the special case of a rank-1 approximation can also be used to correctly estimate matrix 2-norms with very high probability. Our numerical experiments are in full support of our conclusions.

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MS142

Fast Algorithms for the Evaluation of Layer Potentials using 'Quadrature by Expansion'

Quadrature by Expansion, or 'QBX', is a systematic, high-order approach to singular quadrature that applies to layer potential integrals with general kernels on curves and surfaces. This talk discusses algorithmic options for using QBX within a variant of the Fast Multipole Method. A method is presented that preserves accuracy, generality and close evaluation capability while only requiring a relatively modest increase in computational cost in comparison to a point-to-point FMM.

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MS142

Stability and Accuracy of Structured Direct Solvers

Structured direct solvers are known to be very efficient in solving some integral equations and PDEs. Here, we show that they are not only faster than standard direct solvers, but can also have **much better stability**. In particular, for hierarchically semiseparable (HSS) matrices, we first show how the approximation errors can be controlled by the tolerance in either classical or randomized compression. We further demonstrate the backward stability of the direct solution. In fact, the growth of the numerical error in the direct factorization is significantly slower than that in standard LU factorization with pivoting. The growth factors are derived.

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MS143

Fictitious Domain Method with a Hybrid Cell Model for Simulating Motion of Cells in Fluid Flow

This talk will consider a hybrid model to represent biological cells and the distributed-Lagrange-multiplier/fictitious-domain (DLM/FD) formulation for simulating the fluid/cell interactions. The hybrid model to represent the cellular structure consists of a continuum representation of the lipid bilayer, from which the bending force is calculated through energetic variational approach, a discrete cytoskeleton model utilizing the worm-like chain to represent network filament, and area/volume constraints. For our computational scheme, a formally second-order accurate fractional step scheme is employed to decouple the entire system, and is solved by the projection method, level set method, ENO reconstruction, and the Newton method. Numerical results compare favorably with previously reported numerical and experimental results, and show that our method is suited to the simulation of the cell motion in flow.

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MS143

Modeling and Computation of a Precipitate in Inhomogeneous Elastic Media

We present linear theory and nonlinear simulations to study the self-similar growth/shrinkage of a precipitate in a 2D elastic media. For given applied stress boundary conditions, we show that depending on the mass flux entering/exiting the system, there exist critical flux and elasticity at which compact self-similar growth/shrinkage occurs in the linear regime. Numerical results reveal that at long times there exists nonlinear stabilization that leads the precipitate to evolve to compact limiting shape.

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MS143

A Boundary Integral Method for Particles Moving in Viscoelastic Fluids

We present a boundary integral method for computing forces on interacting particles in an unsteady viscoelastic flow. Using a correspondence principle between Stokes flow and linear viscoelasticity in the Fourier domain, we provide a simple boundary integral formulation for solid particles moving in a linear viscoelastic fluid. We present an accurate numerical method for finding the particle surface forces when the velocities are given or vice versa. Our numerical methods are validated against a known exact solution and an existing asymptotic solution. The comparisons are in excellent agreement.

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MS143

Solving Interface Problems to High-order on a Regular Cartesian Grid

In this talk I will present a regular Cartesian grid framework for solving two problem of central importance to interfacial dynamics. The first one is the solution of Poisson's equation with interface jump conditions and the second one is the evolution of the interface. The methods presented are high order (4th order accurate), optimally local (compact stencil sizes), and easy to implement. I will present applications of these methods to solve the incompressible two-phase Navier Stokes equations for flows involving the interaction of droplets with a membrane.

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MS144

Radial Basis Function Collocation Method in Block Pseudospectral Mode

We numerically investigate radial basis function (RBF) collocation method in block pseudospectral (BPS) mode, a method popularized by Driscoll and Fornberg for pseudospectral collocation method. The RBF implementation allows us to deal with irregular domain whereas matching solution and derivatives continuities are done in similar ways as in BPS. Numerical experiments in solving simple collocation problems will be shown.

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MS144

Adaptive Trial Subspace Selection for Ill-Conditioned Kernel Collocation

Choosing data points is a common problem for researchers who employ various meshless methods for solving partial differential equations. On the one hand, high accuracy is always desired; on the other, ill-conditioning problems of the resultant matrices, which may lead to unstable algorithms, prevent some researchers from using meshless methods. In this talk, we will go over some adaptive trial subspace selection algorithms that select basis to approximate the true solution of the full problem.

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MS144

Reproducing Kernel Hilbert Spaces Related to Parametric Partial Differential Equations

Parametric partial differential equations often arise in complicated physical simulations. A recent source for high- and even infinite dimensional problems is the modeling of uncertainties. For the efficient numerical treatment of those problems it is crucial to have a decay in importance of the input parameters. Such a decaying ordering can be formally stated in terms of reproducing kernels. Such a point of view also indicates numerical schemes which are well-known in the kernel-based literature. We will provide some non-standard examples and discuss the resulting approximation properties. This is partly based on joint work with M. Griebel and B. Zwicknagl (both Bonn University).

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MS144

A Novel Radial Basis Function (RBF) Method for Solving Partial Differential Equations (PDEs) on Large Point Clouds

Radial Basis Function (RBF) methods, with advantages such as mesh-free, simplicity of implementation, and dimension-independence, have been broadly employed for reconstructing arbitrary surfaces. However, there are still many challenge problems in the numerical solution of Partial Differential Equations (PDEs) on large point clouds. In this talk, a novel RBF method will be briefly introduced. Several related topics, such as fast algorithms, treecode, will also be discussed. Numerical examples demonstrate that this method yields promising results.

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MS145

Exponentially Decaying Error Rate in One-Bit Compressive Sensing

In one-bit compressive sensing, s-sparse vectors $\mathbf{x} \in \mathbf{R}^n$ are acquired via extremely quantized linear measurements $y_i = \mathrm{sgn}\langle \mathbf{a}_i, \mathbf{x}\rangle$, $i = 1, \ldots, m$. Several procedures to reconstruct these sparse vectors have been shown to be effective when $\mathbf{a}_1, \ldots, \mathbf{a}_m$ are independent random vectors. They typically yield an error decaying polynomially in $\lambda := m/(s \log(n/s))$. This rate cannot be improved in the measurement framework described above. However, we show that a reconstruction error decaying exponentially in λ is achievable when thresholds $\tau_1, \ldots, \tau_m$ are chosen adaptively in the quantized measurements $y_i = \mathrm{sgn}(\langle \mathbf{a}_i, \mathbf{x}\rangle - \tau_i)$, $i = 1, \ldots, m$. Our procedure, which is robust to measurement error, is based on a simple recursive scheme involving either hard-thresholding or linear programming.

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MS145

Compressed Subspace Matching on the Continuum

We consider the general problem of matching a subspace to a set of (compressed) samples. We are interested in the case where the collection of subspaces is continuously parameterized, i.e. uncountably infinite. We present some mathematical theory that shows that a random projection embeds a collection of K-dimensional spaces if the number of samples is on the order of K times a constant that describes the geometry of the collection. We also show how this embedding results in a guarantee on our ability to choose the a subspace which is (almost) as good as the one computed from a full observation of the signal. This is joint work with William Mantzel.

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MS145

Constructing Matrices with Optimal Block Coherence

Block coherence of matrices plays an important role in analyzing the performance of block compressed sensing recovery algorithms (Bajwa and Mixon, 2012). We present bounds on worst-case block coherence and Kronecker product constructions which achieve these bounds. We also show that random subspaces have optimal-order worst-case block coherence asymptotically. Finally, we present a flipping algorithm that can improve the average block coherence of a matrix, while maintaining the worst-case block coherence of the original matrix.

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MS145

Compressed Sensing and Sigma-Delta Quantization: Decoding Via Convex Optimization

We introduce an alternative reconstruction method for signals whose compressed samples are quantized via a Sigma-Delta quantizer. The method is based on solving a convex optimization problem, and unlike the previous approaches, it yields a stable and robust estimate of the original signal. Consequently, we can use Sigma-Delta quantizers for compressible signals and when the measurements are noisy. Finally, our theory applies to "fine" Sigma-Delta quantizers and "coarse" Sigma-Delta quantizers, e.g., 1-bit per measurement.

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MS146

Mori-Zwanzig Analysis of Brownian Motion in a Confined Molecular System

Brownian motion in molecular systems is one of the original examples for which Mori-Zwanzig projection method was developed. Compared to the unbounded case, Brownian motion in a confined fluid exhibits interesting features, which are reflected on its memory kernel. By calculating the memory kernel from molecular dynamics simulations and obtaining analytic results for the Rayleigh gas model, we investigate the effects of confinement.

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MS146

Mori-Zwanzig and Adaptive Mesh Refinement for Uncertainty Quantification

We employ the Multi-element generalized Polynomial Chaos method to deal with stochastic equations involving discontinuities in random space. We develop a new criterion through the model reduction and study the connection between the variances of the outputs and the quantities which are selected as the accuracy control parameters to determine when to carry out the mesh refinement. The Kraichnan-Orszag three mode problem is used to illustrate the effectiveness of the algorithm for ODEs.

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MS146

Scale Dependence and Renormalization in Model Reduction

The problem of model reduction for complex systems is an active area of research. In this talk I want to discuss how the physics inspired concepts of scale dependence and renormalization can be used to facilitate the construction of accurate reduced models for complex problems.

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PP1

A New Test for Exclusion Algorithm to Find the Optimum Value of Function in Rn

The problem of finding the global minimum of a vector function is very common in science, economics and engineering. One of the most notable approaches to find the global minimum of a function is that based on interval analysis. In this area, the exclusion algorithms (EAs) are a well-known tool for finding the global minimum of a function over a compact domain. There are several choices for the minimization condition In this paper, we introduce a new exclusion test and analyze the efficiency and computational complexity of exclusion algorithms based on this approach.We consider Lipschitz functions and give a new minimization condition for the exclusion algorithm. Then we study the convergence and complexity of the method.

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PP1

A Mesh Free Method for Numerical Simulation of Calcium Dynamics In Ventricular Myocytes

We consider a coupled system of non-linear reaction-diffusion equations that model the spatio-temporal variation of intracellular calcium concentration in ventricular myocytes. We introduce a modified mesh free method and utilize exponential time differencing, to significantly reduce the simulation time. At the end we present numerical results demonstrating the stability of the method when used on uneven distribution of nodes.

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PP1

Gene Selection from Microarray Data : An Exploratory Approach

The goal of microarray data analyses is often to identify the smallest set of genes that can distinguish between classes of samples (e.g., from unhealthy samples to healthy ones). In this work, we explore current statistical learning techniques on the discovery of informative genes from microarray experiments. In particular, several gene selection algorithms are tested on a microarray data sets from samples in a type-1-diabetes (T1D) study. The results are compared and discussed.

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PP1

AWM Workshop: Confidence Sets for Geometric and Topological Distances

Distance measures arise in many contexts. Unfortunately, the most interesting distance is the one between an unknown ground truth object and an object created from sampling. In this talk, we introduce the statistical bootstrap for the purpose of bounding the distance between a reconstructed object and the original object. In particular, we derive confidence sets for persistence diagrams, persistence landscapes, road networks, and Reeb graphs.

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PP1

AWM Workshop: Fast Iterative Methods for The Variable Diffusion Coefficient Equation in a Unit

Disk

Variable coefficient diffusion equation has widespread applications in many areas of Engineering and Industrial research like the flow in porous media and Tomography. We present here fast, iterative methods to solve this equation with applications to the Ginzburg Landau equation. Our technique is based on solution of Poisson and Helmholtz equation in a unit disc using fast FFT and recursive relations. The performance of this fast method is illustrated with some numerical examples.

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PP1

Spatiotemporal Pattern of Temperature Change over US Using Bounded-Variation Segmentation

In order to analyze low frequency variability of climate, the method of bounded-variation segmentation is applied for modeling temperature time series of US from 1184 stations during 1900-2012. The method finds multiple linear trends and locate times of significant changes. Important attribute of this method is that it is not dependent on Gaussian or Markovian assumptions. Also multi-dimensional analysis used in this method eliminate the effect of sensors relocation on the detected trends.

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PP1

AWM Workshop: The Asymptotic Analysis of a Thixotropic Yield Stress Fluid in Squeeze Flow

The partially extending strand convection model, combined with a Newtonian solvent, is investigated for a viscoelastic fluid in biaxial extensional (squeeze) flow. For a prescribed tensile stress, the asymptotic analysis, while not simple, is an essential tool for the physical interpretation of the distinct stages in evolution. The overall picture that emerges captures a number of features that are associated with thixotropic yield stress fluids, such as delayed yielding and hysteresis for up-and-down stress ramping.

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PP1

Multiscale Decomposition and Modeling of Complex Networks

Statistical analyses of networks can provide critical insights into the structure, function, dynamics, and evolution of many complex systems. Here, we introduce a flexible method for synthesizing realistic ensembles of networks starting from a known network, through a series of mappings that coarsen and later refine the network structure by randomized editing. The method, MUSKETEER, preserves structural properties with minimal bias, including unknown or unspecified features, while introducing realistic variability at multiple scales.

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PP1

Pathways to Type 2 Diabetes with a Mathematical Model

We develop a mathematical model of how pancreatic beta cells fail in the progression to type 2 diabetes. Insulin resistance by itself does not generally lead to diabetes unless it is extreme. In contrast, typical degrees of insulin resistance do lead to disease if accompanied by an increased propensity to apoptosis, which impairs the ability to expand beta-cell mass or function in response to insulin resistance. We have incorporated the dynamics of exocytosis of insulin granules. These enhancements allow us to look at the mechanistic defects that underlie observed pathologies such as impaired fasting glucose (IFG) and impaired glucose tolerance (IGT). The model supports associations in experiments between IFG and excess HGP and between IGT and peripheral insulin resistance.

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PP1

Bayesian Statistics and Uncertainty Quantification for Safety Boundary Analysis in Complex Systems

The analysis of a safety-critical system often requires detailed knowledge of safe regions and their high-dimensional non-linear boundaries. We present a statistical approach to iteratively detect and characterize the boundaries, which are provided as parameterized shape candidates. Using methods from uncertainty quantification and active learning, we incrementally construct a statistical model from only few simulation runs and obtain statistically sound estimates of the shape parameters for safety boundaries.

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PP1

AWM Workshop: Traveling Fronts to the Combustion and the Generalized Fisher-Kpp Models

We show the nonexistence of traveling fronts in the combustion model with fractional Laplacian $(-\Delta)^s$ when $s \in$

$(0, 1/2]$. Our method can be used to give a direct and simple proof of the nonexistence of traveling fronts for the usual Fisher-KPP nonlinearity. Also we prove the existence and nonexistence of traveling fronts for different ranges of the fractional power s for the generalized Fisher-KPP type model.

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PP1

Which Conical Ant Mound is Optimal in Collection of Solar Beams From Transient Sun

We optimize domes of ant nests, receiving energy from solar heating and losing it to a cold night air. Sun completes the daily sky cycle with beams of radiation continuously changing their altitude and azimuthal angles. We calculate the incoming radiation at each exposed point of a conical dome surface and at each instance from dawn to sunset. The daily energy serves as a criterion and the surface area of the cone, through which heat is lost during night time, serves as an isoperimetric constraint in the sense of Polya-Szego, with the height to cones base ratio chosen as a control variable. For the simplest case, the instantaneous flux of the terrestrial solar power is explicitly expressed through the altitude Sun angle. Time-integration over the azimuthal angle and areal-integration over the illuminated half-cone give the total solar day energy. This functional is then optimized with respect to the size of the anthill that answers the question stated in the title.

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PP1

AWM Workshop: Competitive Geometric Flow Of Network Morphologies Under The Functionalized Cahn-Hilliard (fch) Free Energy

The FCH is a higher order free energy which balances solovation energy of ionic groups against elastic energy of the underlying polymer backbone, and describes the formation of solvent network structures which are essential to ionic conduction in polymer membranes. For the H -1 gradient flow of the FCH energy, using functional analysis and asymptotic methods, we drive a sharp-interface geometric motion which couples the flow of co-dimennsion 1 and 2 network morphologies, through the far-field chemical potential.

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PP1

On a Method for Approximation of the Singularity Curve of a Piecewise Constant Function of Two Variables

We modify the method suggested earlier by us and overcome its main deficiency. The method enables the approximation of the singularity curve of a piecewise constant function of two variables by means of its Fourier-Jacobi coefficients. The method is based on the technique suggested by the author for recovering the locations of discontinuities of a piecewise smooth function of one variable. The method could be generalized for functions of three or more variables. In addition, some numerical examples are presented.

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PP1

Stable Implementation of Complete Radiation Boundary Conditions in Finite Difference Time Domain Solvers for Maxwell's Equations

Complete Radiation Boundary Conditions (CRBCs) allow for the efficient truncation of unbounded domains in wave propagation problems. Unlike standard Perfectly Matched Layer (PML) approaches, CRBCs allow for a weakly time dependent error estimate for both propagating and decaying waves. We demonstrate the how the CRBC can be implemented in a Finite Difference Time Domain (FDTD) scheme and obtain an energy estimate using a summation by parts (SBP) argument to prove stability.

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PP1

Regression in High Dimensions Via Geometric Multi Resolution Analysis

We present a framework for high-dimensional regression using the GMRA data structure. In analogy to classical wavelet decompositions of function spaces, GMRA is a tree-based decomposition of data sets into local affine projections. Moreover, GMRA admits a fast algorithm for computing the projection coefficients on the already-learned dictionary. Within each node of the tree one can also assign regression coefficients in any manner; here we study the simple case of weighted linear regression.

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PP1

Two Projection Methods for Regularized Total Least Squares Approximation

We consider the Total Least Squares problems with Tikhonov Regularization. Since the problem of finding the Total Least Squares solution is equivalent to the solution of the two parameter linear system, our method derives two nonlinear equations from the two parameter linear system,

applied a Newton method with a nonlinear Jacobian matrix that is computed inexpensively. For large-scale problems, this is further combined with two projection methods, one based on bidiagonal reduction, the other projecting onto a generalized Krylov space.

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PP1

Theoretical Analysis of Low-Energy Electron Diffraction: New Results for Real Systems and New Understanding for Model Ones

We describe our novel, first-principles approach to theoretical calculations of low-energy electron diffraction (LEED) spectra, and especially its expansion to off-normal incidence diffraction from few-layer-graphene systems. We compare our calculated off-normal incidence reflection intensities to conventional LEED calculations. We also present an asymptotic investigation of electron scattering in model systems, e.g., 2D square well potential, to better understand the anomalous solutions that create difficulties for our wave-matching approach to this boundary value problem.

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PP1

A Viscoelastic Model That Displays Thixotropic Yield Stress Fluid Behavior

There are biological fluids such as the slime excreted by slugs, which are yield stress fluids. Among them, some are thixotropic. Typically, a model for yield stress fluids begins with inputting a measured value for the yield stress. On the other hand, our model does not assume any yield stress behavior a priori. The relaxation time of the material is taken as a large parameter, and asymptotic solutions are obtained. These display some observed features of thixotropic yield stress fluids.

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PP1

AWM Workshop: Sexual Cannibalism As An Optimal Strategy in Fishing Spiders

We consider a model, based on the aggressive spillover hypothesis, where we link a females propensity to cannibalize a mate to her aggression towards prey. Higher levels of aggression lead to higher food consumption and lower mating rates, a trade-off in fitness. We find an optimal aggression level and analyze its effects on the frequency and type of sexual cannibalism. We then compare our results to existing models of sexual cannibalism.

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PP1

AWM Workshop: Time-Delayed Pdes with Stochastic Boundary in Mathematical Modeling of Kidney

We consider nonlinear time-delayed transport equations with stochastic boundary to study the stability of feedback systems in the kidney. We prove the existence and uniqueness of the steady- state solution for deterministic and stochastic boundary cases with small delay, based on the contraction mapping theorem. Model results revealed that the system admits the stationary solution for small delay despite stochastic influences, whereas it exhibits oscillatory solutions for large delay, resembling irregular oscillations in spontaneously hypertensive rats.

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PP1

Analysis of a Camera-Based Model of Bar Code Decoding

This work addresses the issue of the limited capability of a camera-based bar code decoding method. The question we wish to address is "What is the resolution needed in the captured image to unambiguously decode a bar code?" For simplicity, we consider the UPC bar code which consists of black and white bars of different widths. The width of the black and white bars encode a 12-digit number according to a look-up table. The smallest element in the bar code is assumed to be of width h. We further assume that the camera pixels are lined up along the bars and they are of size d. The question now amounts to unique determination of the digits for a fixed ratio of d to h. We show that the digits are uniquely determined if the pixel size is no greater than twice the smallest element. Moreover, we show that this determination is stable. A decoding algorithm is presented, along with numerical examples that illustrate the main ideas behind this work.

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PP1

Fully Nonlinear Model for Dispersive Wave Turbulence

The Majda-McLaughlin-Tabak (MMT) model describes a one-dimensional system exhibiting dispersive wave turbulence, and includes linear and nonlinear terms. I consider a modified version of the model where the linear term is absent. I discuss symmetry-based arguments, perturbative solutions, and other methods for predicting the dispersion relation and waveaction spectrum, and compare with numerical results. I consider both the case where driving and damping are present and the case where they are absent.

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PP1

Ritz-Augmented Extended Krylov Subspaces for Sequences of Lyapunov Equations

We consider the numerical solution of generalized Lyapunov equations occurring in bilinear model order reduction. We proceed by splitting the operator and use a classical stationary iteration, performing standard Lyapunov solves with the extended Krylov subspace method. This enables reuse of computation via the use of augmented Krylov subspaces. The resulting algorithm appears competitive with the existing state of the art on two benchmark problems.

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PP1

Numerical Investigation of Microfluidic Droplet Breakup Using T-Junction Geometry

A critical analysis on the breakup of Microfluidic droplet in a T-junction is presented. A way by which droplets can be evenly distributed over multiple micro channels is to break them into many smaller droplets. Hence it is essential to understand the behavior of the breakup of droplet in a micro channel. Available theoretical and numerical data are compared with simulations obtained using a modified version of the interFoam solver of the OpenFOAM CFD package.

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PP1

A Mathematical Model of Moisture Movement and Bacterial Growth in a Two-Dimensional Porous Medium

Bacterial growth in sand is of concern in regard to the health of beaches. A mathematical model is presented that represents the movement of moisture and the growth of bacteria through a beach. Simulations were run by numerically solving Richard's Equation using a Finite Volume Method. These simulations show that elevated bacteria counts following rain events do not necessarily result from bacteria in the body of water, but can also be sourced from the sand.

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PP1

A Guaranteed, Adaptive, Automatic Algorithm For Univariate Function Minimization

This algorithm attempts to provide an approximate minimum value of a one-dimensional function that differs from exact minimum value by no more than an error tolerance. Besides guaranteed the error tolerance, this algorithm also considers the lengths tolerance of the subset containing point(s) where the minimum occurs.

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PP1

Iterative Functional Modification Method for Solving a Transportation Problem

New method for solving transportation problems based on decomposing the original problem into a number of two-dimensional optimization problems is proposed. Since the solution procedure is integer-valued and monotonic in the objective function, the required computation is finite. As a result, we get not only a single optimal solution of the original transportation problem but a system of constraints that can yield all optimal solutions. We give numerical examples illustrating the constructions of our algorithm.

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PP1

A Multiscale Implementation for the Peridynamic Model of Mechanics

An investigation in continuous and discontinuous finite element methods for a peridynamics model of mechanics gives us a new view of the peridynamic model when dealing with solutions with jump discontinuities. Peridyanmics can be transit between nonlocal and local models depending on the size of horizon compared to the grid size. Therefore, a mesh of good quality and an appropriate quadrature rule to conform the multiscale setting need to be concerned. We developed a local grid refinement method that can be suitable for the multiscale peridynamic model and also found a quadrature rule to estimate the weak formulation with high accuarcy.

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PP1

AWM Workshop: Three Model Problems for 1-D Particle Motion with the History Force in Viscous Fluids

Abstract. We consider various model problems that describe rectilinear particle motion in a viscous fluid under the influence of the history force. These problems include sedimentation, impulsive motion, and oscillatory sliding motion. The equations of motion are integrodifferential equations with a weakly singular kernel. We provide analytical solutions using Laplace transforms and discuss the mathematical relation between the sedimentation and impulsive start problems. We also compare several numerical schemes and benchmark them against the analytical results.

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PP1

AWM Workshop: A Local Grid Mesh Reinement for a Nonlocal Model of Mechanics

Nonlocal problems are based on integro-diferential equations, which do not involve spatial derivatives. This makes it possible to deal with discontinuous solutions. We are most interested in the numerical results for piecewise solutions with a jump discontinuity. A local grid reinement method is then investigated for two-dimensional nonlocal model, which would be suitable for the curve discontinuous path. With the reine meshes, optimal convergence behaviors are achieved.

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PP1

Designing a Self-Propelled Hydrogel Microswimmer

We use dissipative particle dynamics to design a new self-propelling bi-layered gel microswimmer. The gel consists of one layer that swells in response to an external stimulus and one passive layer. When a periodic stimulus is applied, the microswimmer undergoes a sequential expansion, bending, contraction, and straightening motions leading to net propulsion at low Reynolds number. We probe how the swimming speed can be enhanced by selecting material properties and geometry of the gel swimmer.

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PP1

Inverse Modeling and Prediction Uncertainty Analysis of a Co2 Injection Pilot Test, Cranfield, Mississippi

The ensemble-based filtering algorithms and the null-space Monte Carlo approach are applied for characterizing the heterogeneity and quantifying model prediction uncertainty of a CO2 injection test, Cranfield, Mississippi. An ensemble of reservoir model conditioned to the observed data is retained from both approaches and models prediction results are analyzed to evaluate the trade-off between model efficiency and model complexity to provide a computationally efficient and practically useful framework for predictive uncertainty analysis of CO2 sequestration.

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PP1

A Spatio-Temporal Point Process Model for Ambulance Demand

We model spatio-temporal point processes as a time series of spatial densities using finite mixture models. We fix the mixture component distributions across time while letting the mixture weights evolve over time. We capture seasonality by constraining mixture weights; we represent location-specific temporal dependence by applying autoregressive priors on mixture weights. To illustrate, we estimate ambulance demand in Toronto, Canada. Our method accurately captures the complex spatial and temporal dynamics present in this large-scale dataset.

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