AN12 and FM12 Abstracts

2012 SIAM ANNUAL MEETING

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1952 – 2012

July 9–13

SIAM Conference on

Financial Mathematics & Engineering

July 9-11, 2012
Hyatt Regency Minneapolis
Minneapolis, Minnesota, USA

Abstracts are printed as submitted by the authors.

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AN12 Abstracts

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IC1

On the Shape of Data

Topology is the mathematical discipline which studies shape. Data sets typically come with a notion of distance which formalizes notions of similarity of data points. The shape of the data is of a great deal of importance in understanding it - cluster decompositions define subpopulations of the data and presence of loops often is a clue to the presence of periodic or recurrent behavior in it. In this talk, we will describe how topological methods can be adapted to the study of data sets, with examples.

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IC2

Elliptic Curve Cryptography and Applications

In the last 25 years, Elliptic Curve Cryptography has become a mainstream primitive for cryptographic protocols and applications. This talk will give a survey of elliptic curve cryptography and its applications, including applications of pairing-based cryptography which are built with elliptic curves. No prior knowledge about elliptic curves is required for this talk. One of the information-theoretic applications I will cover is a solution to prevent pollution attacks in content distribution networks which use network coding to achieve optimal throughput. One solution is based on a pairing-based signature scheme using elliptic curves. I will also discuss some applications to privacy of electronic medical records, and implications for secure and private cloud storage and cloud computing.

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IC3

Applying Mathematics to Better Understand the Ocean

The ocean still represents a realm of discovery in many important respects. We do not, for example, fully understand the magnitude of mixing in the ocean, and this lack of knowledge has real consequences for our ability to model and predict future climate. In this talk I will describe how we have been using ideas from dynamical systems to bring a new degree of clarity to this problem. I will discuss how this has improved our theoretical understanding of some of the key processes driving ocean circulations and how we have been literally applying mathematics to the ocean by deploying floats in the Southern Ocean to map unstable manifolds and calculate Lyapunov exponents.

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IC4

Image Processing and Computational Mathematics

Image processing has traditionally been studied as a form of signal processing, and a subfield of electrical engineering. Recently, with the advent of inexpensive and integrated image capturing devices, leading to massive data and novel applications, the field has seen tremendous growth. Within computational mathematics, image processing has emerged not only as an application domain where computational mathematics provide ideas and solutions, but also in spurring new research directions (a new Computational Fluid Dynamics) in geometry (Total Variation regularization and Level Set methods), optimization (primal-dual, Bregman and Augmented Lagrangian methods, L1 convexification), inverse problems (inpainting, compressive sensing), and graph algorithms (high-dimensional data analysis). This talk gives an overview of these developments.

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IC5

Model-Assisted Effective Large Scale Matrix Computations

Advanced mathematical models very often require the solution of (sequences of) large algebraic linear systems, whose numerical treatment should incorporate problem information in order to be computationally effective. For instance, matrices and vectors usually inherit crucial (e.g., spectral) properties of the underlying continuous operators. In this talk we will discuss a few examples where the performance of state-of-the-art iterative linear system solvers can be dramatically enhanced by exploiting these properties. Our presentation will focus on structured linear systems stemming from the numerical discretization of systems of partial differential equations, as well as of optimal control problems constrained by partial differential equations.

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IC6

Multiscale Problems Involving Disorder: A Mathematical Perspective

The talk will review a series of recent works, including works in collaboration with X. Blanc, F. Legoll, PL. Lions addressing various aspects, both mathematical and numerical in nature,of some multiscale problems involving non periodic and random modelling. The problems considered all originate from materials science at different scales. The common motivation of the approaches presented is the wish to keep the computational workload as limited as possible, despite the presence of disorder (non periodicity, defects, randomness) in the problems.

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IC7

Freeform Architecture and Discrete Differential Geometry

The emergence of freeform structures in contemporary architecture raises numerous challenging research problems many of which are related to the actual fabrication and are of a mathematical nature. The speaker will report on recent progress in geometric computing for freeform architecture, with special emphasis on the close relation to discrete differential geometry. Specific topics to be addressed include: meshes with planar quadrilateral faces and corresponding supporting structures, semi-discrete representations for structures from single curved panels, paneling algorithms and the design of self supporting surfaces. The transfer of research into the architectural practice will be illustrated at hand of selected projects.

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IC8

Computing Essentials: What SIAM Members Should Know About Emerging Architectures

For most of computing history programmers have experienced steady performance improvement with little effort, primarily due to increased clock speed and instruction level parallelism: Riding the commodity performance curve was easy. This has changed. Multicore and GPU processors promise terascale laptop, petascale deskside and exascale center systems. But realizing this potential is challenging: Riding the new commodity performance curve requires parallel execution. Furthermore, the number of components in high-end systems will increase soft and hard system errors. We discuss the essentials of how to develop algorithms and software in order to realize parallel performance today and prepare for the future.

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IC9

Overcoming the Tyranny of Scales in Subsurface Flow and Reactive Transport Simulation

A grand challenge facing subsurface modelers is the disparity between length and time scales at which fundamental processes are controlled and those at which predictions are needed. This presentation will describe the application of multiscale simulation methods to this challenge. Particular focus will be given to 1) hybrid multiscale simulations, which directly couple pore- and continuum-scale models, and 2) integration of genome-scale microbial metabolism models into field-scale bioremediation analyses. We will present our multiscale analysis platform (or MAP), a community resource for navigating the breadth of multiscale methods and identifying which tools are best suited to specific problems.

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IC10

Network Formation and Ion Conduction in Ionomer Membranes

Selective charge transport is an essential step in efficient energy conversion. Ionomer membranes are formed from cross-linked, charged polymers. They imbibe solvent to form nanoscaled network structures which lie at the heart of many energy conversion devices. Experimental data shows that the networks are hysteretic, evolving on time scales of minutes and hours, far outside the reach of molecular simulations. We present a novel reformulation of the classical Cahn-Hilliard free energy that permits the inclusion of solvation energy and counter-ion entropy within a continuum model. Gradient flows on the Functionalized Cahn-Hilliard energy show bi-stability of bilayer, pore, and micelle dominated networks. We present sharp interface reductions, including classes of curvature driven flows that couple to the network structure.

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IP1

On Mean Field Games

This talk will be a general presentation of Mean Field Games (MFG in short), a new class of mathematical models and problems introduced and studied in collaboration with Jean-Michel Lasry. Roughly speaking, MFG are mathematical models that aim to describe the behavior of a very large number of agents who optimize their decisions while taking into account and interacting with the other agents. The derivation of MFG, which can be justified rigorously from Nash equilibria for N players games, letting N go to infinity, leads to new nonlinear systems involving ordinary differential equations or partial differential equations. Many classical systems are particular cases of MFG like, for example, compressible Euler equations, Hartree equations, porous media equations, semilinear elliptic equations, Hamilton-Jacobi-Bellman equations, Vlasov-Boltzmann models... In this talk we shall explain in a very simple example how MFG models are derived and present some overview of the theory, its connections with many other fields and its applications.

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IP2

Complex Adaptive Systems and the Challenge of Sustainability

The continual increase in the human population, magnified by increasing per capita demands on Earth's limited resources, raise the urgent mandate of understanding the degree to which these patterns are sustainable. The scientific challenges posed by this simply stated goal are enormous, and cross disciplines. What measures of human welfare should be at the core of definitions of sustainability, and how do we discount the future and deal with problems of intra-generational and inter-generational equity? How do environmental and socioeconomic systems become organized as complex adaptive systems, and what are the implications for dealing with public goods at scales from the local to the global? How does the increasing interconnectedness of coupled natural and human systems affect the robustness of aspects of importance to us, and what are the implications for management. What is the role of social norms, and how do we achieve cooperation at the global level? All of these issues have parallels in evolutionary biology, and this lecture will explore what lessons can be learned from ecology and evolutionary theory for addressing the problems posed by achieving a sustainable future.

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IP3

The Isoperimetric Problem Revisited: Exposing Eulers 1744 Proof of Necessity as a Proof of Sufficiency, as Such the First and Shortest in History

In this talk the speaker will outline the remarkable life of the isoperimetric problem (Determine, from all simple closed planar curves of the same perimeter, the one that encloses the greatest area) and argue that it has been the most influential mathematics problem of all time. In 1744 Euler constructed multiplier theory to solve the isoperimetric problem; however he concluded that his theory was only necessary and not sufficient to prove that the circle was the solution. Some 130 years later Weierstrass constructed his elegant sufficiency theory for problems in the calculus of variations and used it to give the first complete proof that the circle solved the isoperimetric problem. The speaker will demonstrate that Eulers original proof was merely an observation away from establishing sufficiency. As such it should be viewed as the first and shortest solution to the isoperimetric problem in history.

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IP4

Complex Networks. A Tour d' Horizon

The field of complex network is gently introduced. The classical concepts of small-world and scale-freeness are briefly discussed. Then, the problem of communicability in complex networks is motivated and analyzed by considering the use of matrix functions. The concept of network communicability is then applied to a few real-world situations. It motivates a new Euclidean metric for networks, which allows to embed every network into a hypersphere of certain radius. Finally we discuss dynamical processes on networks. In particular we show how to extend these concepts to the consideration of long-range interactions among the agents in complex networks. The consequences of these extensions for real-world situations are briefly discussed.

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IP5

Linear Algebra Methods for Data Mining with Applications to Materials Science

The field of data mining is the source of many new, interesting, and sometimes challenging, linear algebra problems. In fact, one can say that data mining and machine learning are now beginning to shape a "new chapter" in numerical linear algebra. We will illustrate the key concepts and discuss dimension reduction methods which play a major role in machine learning. The synergy between high-performance computing, efficient electronic structure algorithms, and data mining, may potentially lead to major discoveries in materials. We will report on our first experiments in 'materials informatics', a methodology which blends data mining and materials science.

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IP6

Multifidelity Modeling for Identification, Prediction and Optimization of Large-scale Complex Systems

Often we have available several numerical models that describe a system of interest. These numerical models may vary in "fidelity" or "skill," encompassing different resolutions, different physics, and different modeling assumptions; they may also include surrogates such as reduced-order models. A multifidelity approach seeks to exploit optimally all available models and data. This talk discusses the key elements of multifidelity modeling: constructing reduced-order models, quantifying model uncertainties, selecting models with appropriate fidelity for the prediction/decision task at hand, and synthesizing multifidelity information. We show the benefit of multifidelity modeling for the tasks of prediction, design optimization, and uncertainty quantification.

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SP1

AWM-SIAM Sonia Kovalevsky Lecture: The Role of Characteristics in Conservation Laws

Sonya Kovalevsky, in the celebrated Cauchy-Kovalevsky theorem, made clear the significance of characteristics in partial differential equations. In the field of hyperbolic conservation laws, characteristic curves (in one space dimension) and surfaces (in higher dimensions) dominate the behavior of solutions. Some examples of systems exhibit interesting, one might even say pathological, characteristic behavior. This talk will focus on ways that characteristics in systems of conservation laws give information about the systems being modeled.

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SP2

The John von Neumann Lecture: Liquid Crystals for Mathematicians

Liquid crystals form an important class of soft matter systems with properties intermediate between solid crystals and isotropic fluids. They are the working substance of liquid crystal displays, which form the basis of a huge multinational industry. The lecture will describe these fascinating materials, and what different branches of mathematics, such as partial differential equations, the calculus of variations, multiscale analysis, scientific computation, dynamical systems, algebra and topology, can say about them.

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SP3

Past President's Address: Reflections on SIAM, Publishing, and the Opportunities Before Us

Upon taking up the post of president I had, of course, formulated my priorities for SIAM. This talk provides a good occasion to revisit some of those. One area turned out to play a vastly larger role than I would have anticipated, namely mathematical publishing and many issues associated with it, ethical, technological, economic, political, and scientific. The future of scholarly publishing is far from clear, but one thing seems certain: big changes are needed and will be coming. We, as mathematicians, are major stakeholders. We should also be major agents in guiding these changes. I will present some of my observations and thoughts as we confront the opportunities before us.

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SP4

W. T. and Idalia Reid Prize Lecture: Large Algebraic Properties of Riccati Equations

In the eighties there was considerable interest in the algebraic properties of the following Riccati equation

$$A^*X + XA - XBB^*X + C^*C = 0, \quad (1)$$

where $A, B, C \in A$, a Banach algebra with identity, and the involution operation $*$. Conditions are sought to ensure that the above equation has a solution in A. The results were disappointing and the problem was forgotten until this century when engineers studied the class of spatially distributed systems. One application was to control formations of vehicles where the algebraic property was essential. This case involves matrices A, B, C with components in a scalar Banach algebra. Positive results are obtained for both commutative and noncommutative algebras.

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SP5

I.E. Block Community Lecture: Creating Reality: The Mathematics Behind Visual Effects

Film-makers have long realized one of the best ways to convince audiences that a computer-generated effect, like a stormy ocean, is real is to numerically solve physical equations describing the motion, bringing mathematics and scientific computing into the forefront of animation. As we progress to solving more physics more accurately and faster, a whole new way of working has emerged, "virtual practical effects", where artists set up shots virtually as they'd want to in the real world and let simulated physics take over. I'll demonstrate how a little mathematical analysis can make a world of difference to making a film.

Robert Bridson
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JP1

Systemic Risk

What is systemic risk, how do we model it,how to we analyze it, and what are the implications of the analysis? I will address these issues both in a larger historical context and within current research mathematical finance. The key property of systems subject to systemic risk is their inter-connectivity and the way individual risk can become overall, systemic risk when it is diversified by inter-connectivity. I will discuss theoretical issues that come up with mean-field and other models and will also show results of numerical simulations.

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CP1

A-Posteriori Verification of Optimality Conditions for Control Problems with Finite-Dimensional Control Space

In this paper we investigate non-convex optimal control problems.We are concerned with a-posteriori verification of sufficient optimality conditions.If the proposed verification method confirms the fulfillment of the sufficient condition then a-posteriori error estimates can be computed. A special ingredient of our method is an error analysis for the Hessian of the underlying optimization problem.We derive conditions under which positive definiteness of the Hessian of the discrete problem implies positive definiteness of the Hessian of the continuous problem.The article is complemented with numerical experiments.

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CP1

Modeling and Control of Nanoparticle Delivery to Tumor Sites with Experimental Validation

Currently, experimental trials are underway to investigate the therapeutic bioavailability of nanoparticles used in the treatment of certain types of cancers. This presentation will discuss the development of mathematical models to predict and controls to regulate the concentration of such nanoparticles in a mammalian body post-injection. The elimination of nanoparticles from the blood and into targeted tumors and the reticulo-endothelial system will be evaluated.

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CP1

Discrete Approximations of Controlled Stochastic Systems with Memory

This paper considers discrete approximations of an optimal control problem in which the controlled state equation is described by a general class of stochastic functional differential equations with a bounded memory. Three different approximation methods, namely (i) semidiscretization scheme; (ii) Markov chain approximation; and (iii) finite difference approximation, are investigated.

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CP1

Steady State Sets of Non-Linear Discrete-Time Control Dynamical Systems with Singular Disturbance

Finding steady state sets is an important topic in the study of dynamical systems. In this paper, we concentrate our efforts to non-linear discrete-time control dynamical systems with large singular disturbance that are modeled by multiple valued iterative dynamical systems or set valued dynamical systems. Because the traditional means of calculus usually fails under the extensive influence of singularity, the use of alternative methods such as multiple valued iterative dynamics modeling is necessary in general. Under the multiple valued iterative dynamics modeling, the steady state sets of non-linear discrete-time control dynamical systems turn out to be the locally maximal strongly full-invariant sets, and we discuss how to reach it in countable steps so that the finite step approximation problem is well posed. We also discuss the invariant fractal structure that often arises due to the large singular disturbance.

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CP1

Sparsity-Promoting Optimal Control of Distributed Systems

We design sparse and block sparse feedback gains that minimize variance amplification of distributed systems. We first identify patterns that strike a balance between the quadratic performance and controller sparsity. We then optimize the feedback gains subject to the structural constraints determined by the identified sparsity patterns. We employ the alternating direction method of multipliers and exploit structure of sparsity-promoting terms to decompose the minimization problem into sub-problems that can be solved analytically.

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CP1

Exact Controllability of the Linear Advection Equation with Interior Controls

An exact controllability result is discussed for the following controlled linear advection equation:

$$\begin{aligned} &\rho_t + \bigtriangledown \cdot (\vec{f}\rho) = \chi_A(x)u(x,t), \\ &\rho(x,0) = \rho_0(x); \rho|_{\Gamma_i} = 0, \end{aligned} \tag{2}$$

where ρ is the state, $u(x,t) \in L^2([0,\tau]; A)$ is the control input, $\vec{f}(x)$ is a smooth vector field, $\Gamma_i \subset X$ is the inflow portion of the boundary ∂X, and $\rho_0(x)$ is the initial state. The result states that the region of controllability in time τ is the portion of X that is touched by solutions of the ODE $\dot{x} = f(x); x(0) = x_0$ in time τ emanating from initial points $x_0 \in A$. An explicit expression for the controllability (and by duality, the observability) gramian is shown, and some ideas to use the gramians for optimal placement of actuators and sensors will be discussed.

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CP1

Solving Optimal Control Problems with Control Delays Using Direct Transcription

Numerical solutions of optimal control problems with delays are important in industry. Solutions to these types of problems are difficult to obtain via analytic techniques. Direct Transcription is a popular numerical method used to compute the solutions of optimal control problems. In this paper we report on the progress and challenges of developing a general purpose industrial grade direct transcription code that can handle problems with both state and control constraints and delays.

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CP2

A Discrete Dynamical Systems Model to Study the Interaction Between Arctic Sea-Surface Temperature and Sea-Ice Cover

We propose a mathematical model involving discrete dynamical systems to understand the interaction between sea-surface temperature and sea-ice cover over the Arctic Ocean. In particular, we use ideas from dynamical systems such as bifurcations and basins of attraction of equilibria along with basic probability theory to make future projections about the possibility of extinction of Arctic sea-ice cover, one of the top five tipping points in the Earth's climate. Observed data from multiple sensors will be used to validate the model. The implications and caveats of the future projections made by our model will be explored.

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CP2

Numerical Studies of Eor by Asp-Flooding

Of the new techniques leading to increase oil production, EOR, which uses chemical additives, is one of the most promising. Chemical flooding is a way to recover additional oil after water-flooding. It involves adding sufficient amounts of chemical species to injected fluids to change phase properties in a way that will enhance oil recovery. However, it is still a big problem that how to appropriately choose the displacing fluids based on their properties and the sequence in which these should be injected to produce oil out as much as possible. In this talk, we will present our results for optimal profiles on Polymer-Water flooding as well as Alkaline-Surfactant-Polymer-Water flooding. It will be discussed for the cases of constant and variable concentrations of injected chemicals. The research reported here has been made possible by a grant NPRP 08-777-1-141 from the Qatar National Research Fund (a member of The Qatar Foundation). The statements made herein are solely responsibility of the authors.

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CP2

Bregman Iterations for Geosounding Inversion

A novel algorithm for nonlinear inversion based on Bregman iterations is applied to electrical, electromagnetic and resistivity soundings. Tikhonov's inversion method, commonly employed for solving inverse problems solving, produces smooth, "smeared" models. Several techniques have been proposed in order to improve the model development in layered models, particularly in geophysics. Some change the norm to L1 or total variation, and others propose a piecewise-continuous model. In the case of L1 optimization, a computationally expensive solver is required. Bregman iterative method has recently proposed for L1 minimization problems, particularly when a sparse representation is required. An iterative, coordinate descent method is implemented based on Bregman distance. Results for several data of electrical, electromagnetic and resistivity soundings are presented.

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CP2

High Frequency Acoustic Propagation Using Level Set Methods

We discuss an application of the level set method to underwater acoustic propagation. The level set model provides a way to compute acoustic wavefronts on a fixed grid, so that the user has more control over the accuracy of the final solution than with the standard Lagrangian approaches (i.e., ray tracing). The method includes high order numerical boundary conditions for reflections from hard surfaces and allows for arbitrary, range-dependent sound speed data as input.

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CP2

How Do You Determine Whether The Earth Is Warming Up?

How does one determine whether the extreme summer temperatures in Moscow of a few years ago was an extreme climatic fluctuation or the result of a systematic global warming trend? It is only under exceptional circumstances that one can determine whether a climate signal belongs to a particular statistical distribution. In fact, climate signals are rarely "statistical;" other than measurement errors, there is usually no way to obtain enough field data to produce a trend or tendency, based upon data alone. We propose a trend or tendency methodology that does not make use of a parametric or statistical assumption. The most important feature of this trend strategy is that it is defined in very precise mathematical terms.

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CP2

An Adaptive Strategy with Unconditional Convergence for Solving Nonlinear Coupled Flow and Transport Equations in Porous Media

We propose a new hybrid strategy for solving flow and transport equations in porous media . At each iteration, after updating pressure from a reduced system of linear equations, we decompose the phases flow graph into its strongly connected components. Saturation field is updated by traversing the resulting graph from upstream to downstream. We update pressure and saturation simultaneously in counter current flow regions identified by multicell components to resolve the tight coupling. The results show that the algorithm is convergent for very large time step sizes.

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CP2

Use of Integral Transforms in Analyzing Nmr Data

In Nuclear Magnetic Resonance (NMR) applications to study porous media, the measured data is modeled as a Laplace transform of the probability density function (PDF) of relaxation times. In this presentation, we describe a novel method to directly compute linear functionals of the PDF without computing the PDF. This method involves a linear transform of the measured data using integral transforms. Different linear functionals of the PDF can be obtained by choosing appropriate kernels in the integral transforms.

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CP3

An Object-Oriented Linear System Solver for Matlab

The MATLAB backslash is an elegant interface to a suite of high-performance methods for solving linear systems and least-squares problems. However, its simplicity prohibits the reuse of its factorization for subsequent systems. Naive MATLAB users also have a tendency to translate mathematical expressions from linear algebra directly into MATLAB, so that $x = A^{-1}b$ becomes the unfortunate x=inv(A)*b. To address this problem, an object-oriented factorize method is presented. Via operator overloading, solving two linear systems can be written as F=factorize(A); x=F\b; y=F\c, where A is factorized only once. The selection of the best factorization method is hidden from the user. The expression $x = A^{-1}b$ translates into x=inverse(A)*b, without computing the inverse.

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CP3

Sign Patterns That Allow Strong Eventual Nonnegativity

A sign pattern is potentially eventually nonnegative (potentially strongly eventually nonnegative) if there is a matrix with this sign pattern that is eventually nonnegative (eventually nonnegative and has some power that is both nonnegative and irreducible). The study of potentially eventually nonnegative sign patterns is hindered by nilpotent matrices and matrices which have powers that are reducible with a nilpotent diagonal block. This talk presents results about potentially strongly eventually nonnegative sign patterns.

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CP3

Matrix Computation and Its Application to Signal Processing

First part of this presentation aims to leverage computing of the determinant of a 3×3 matrix whose ith row is defined by [$a_1{}^i + a_2{}^i + a_3{}^i \quad a_1{}^{i-1} + a_2{}^{i-1} + a_3{}^{i-1} \quad a_1{}^{i-2} + a_2{}^{i-2} + a_3{}^{i-2}$] without expanding. Second part of this presentation is the application to signal processing, specifically to non-uniform sampling [Yih-Chyun Jenq, Perfect Reconstruction of Non-Uniformly Sampled Signal, IEEE Trans. Inst.&Meas. 1997].

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CP3

Classification of Potentially Eventually Exponentially Positive Sign Patterns of Small Order

A matrix A is *eventually exponentially positive* if there exists a positive real number t_0 such that for all $t \geq t_0, e^{tA} > 0$. A *sign pattern* is a matrix having entries in $\{+, -, 0\}$. A sign pattern $\mathcal{A}$ is *potentially eventually exponentially positive* (PEEP) if there exists a matrix A in the qualitative class of $\mathcal{A}$ such that A is eventually exponentially positive. A classification of all 2x2 and 3x3 PEEP sign patterns is given.

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CP3

Positive Semidefinite Zero Forcing

The zero forcing number $Z(G)$ is used to study the maximum nullity/minimum rank of the family of symmetric matrices described by a simple, undirected graph G. We study the positive semidefinite zero forcing number $Z_+(G)$ and some of its properties. In particular, we determine the maximum positive semidefinite nullity and positive semidefinite zero forcing number for a number of graph families appearing in the AIM minimum rank graph catalog.

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CP3

On Estimating Hitting and Commute Times for Large Dense Digraphs

Recent studies have established that the lengths of random-commutes between a source-destination pair, in large dense undirected-graphs, can be well approximated in terms of scaled degrees of the end-point vertices, which implicates the relevance of commute times as a distance in machine learning tasks. In this work we generalize the approximations to strongly connected directed-graphs, albeit in terms of the steady-state-stationary-probability distribution. In so doing, we develop a theoretical framework for these approximations, without resorting to the interplay between undirected graphs and electrical-networks, an analogy on which previous studies rely and, more importantly, one that does not apply to directed-graphs.

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CP4

Contour Detection and Completion for Inpainting and Segmentation Based on Topological Gradient and Fast Marching Algorithms

We combine the topological gradient, a powerful method for edge detection in image processing, and a minimal path method in order to find connected contours. The topological gradient provides a more global analysis of the image than the standard gradient, and identifies the main edges. Then the fast marching algorithm identifies minimal paths in the topological gradient image. This coupled algorithm quickly provides accurate and connected contours. We present applications to inpainting and segmentation.

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CP4

Iterative Wavefront Reconstruction in Adaptive Optics

Obtaining high resolution images of space objects from ground based telescopes is challenging, and often requires computational post processing using image deconvolution methods. Good reconstructions can be obtained if the convolution kernel can be accurately estimated. The convolution kernel is defined by the wavefront of light, and how it is distorted as it propagates through the atmosphere. We describe the wavefront reconstruction problem - a new linear least squares model that exploits information from multiple measurements.

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CP4

Parallel Markov Chain Monte Carlo Methods in Optical Tomography

Markov Chain Monte Carlo (MCMC) is a standard sampling method in Bayesian inference. However, it is slow because it requires that the forward model is solved at every iteration. Furthermore, the standard algorithm is inherently sequential. We will discuss successful parallelization techniques involving a single and a multiple chains method that both shorten computations and improve sample quality. We will then show results from applying them to a real-world, optical tomography problem.

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CP5

Using An Old Traffic Flow Model to Gain New Insights into a Biological Process

The use of a nonlinear PDE to model the elongation process on ribosomal RNA is discussed. Experimentally, the motion of a transcription complex experiences multiple pauses, and the density of elongating complexes may be sufficiently high to experience traffic jams. The traffic flow model includes the presence of non-uniform distributions of pauses along the rrn operon and is used to estimate the instantaneous elongation rate. Discontinuous Galerkin methods are used for the model simulations.

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CP5

Interior-Point Methods for An Optimal Control Influenza Model

We introduce a discrete optimal control problem in order to minimize the number of infected individuals on a single influenza outbreak. We evaluate the effect of social distancing and antiviral treatment as control policies. We solve the problem by using Forward-Backward and Interior-Point Method. Our simulations show that Interior point method gives more robust results than Forward-Backward method. Finally we introduce an isoperimetric constraint to consider limited resources.

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CP5

Modeling the Effect of a New Antibiotic on the Transmission of Antimicrobial Resistant Bacteria in a Hospital Setting

The increase in antibiotic resistance continues to pose a public health risk as very few new antibiotics are being produced, and the prevalence of bacteria resistant to currently prescribed antibiotics is growing. In this talk, we use both deterministic and stochastic mathematical models to analyze the benefits and limitations of the introduction of a new antibiotic in both a large hospital setting and a smaller unit within a hospital under different administration protocols.

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CP5

Modeling Behavior: Using Game Theory and Population Modeling to Explain Sub-Maximal Parasitism

We examine the implications of spatial structure on the evolution of parasitism rates for a well-characterized interaction between a parasitoid wasp and host butterfly on a fragmented landscape. We present multiple evolutionary hypotheses, formulated as mathematical models, and show the extent to which landscape features (patch quality, density, and connectedness) and host attributes (dispersal ability, reproductive success, mortality) affect the viability of this mechanism; thus unveiling the role of spatial processes in the interaction.

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CP6

Modeling Cell Movement Through Collagen Using the Level Set Method

Cell movement affects different biological processes. In the body, cells move through a three-dimensional network of collagen, filaments, and other proteins. We are modeling cell movement through a series of deformable obstacles representing this network. We use the level set method to track the membrane of the cell and borrow concepts from the theory of beams to model the network. Our goal is to use the simulations to model the environment within the body and to investigate variations of this environment on cell movement.

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CP6

A Sparse Update Method for the in-Silico Manipulation of Biological Signaling Pathways

Radon Institute for Computational and Applied Mathematics Austrian Academy of Sciences Defective biological signaling pathways are linked to various pathological conditions and the correction of dysfunctional qualitative behaviour such as oscillation or bistability is a major goal of pharmaceutical and clinical research. Based on differential equation models of the underlying biochemical reaction networks we formulate nonlinear inverse problems and suggest a sparse update algorithm that determines a comprehensible number of candidate network intervention sites. The practicability of our approach is demonstrated by an example related to defective apoptotic signaling.

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CP6

An Unbiased Estimator of Noise Correlations un-

der Signal Drift

Estimation of correlations in noises is important in large-scale modeling and data analysis. In neuroscience, small correlations in noises (trial-to-trial response variations) can decrease coding capacity by sensory neurons dramatically. Although significant noise correlation has been reported from almost all cortical areas, nonstationarity, such as a drift in signals (mean responses) might engender artificial correlations even if no actual correlation exists. Although attempts to estimate noise correlation under changing environments have been made, they were useful only for specific cases. This study presents consideration of a bivariate normal distribution for activities of two neurons and advances the proposition of a semiparametric method for estimating its covariance matrix in an unbiased fashion, whatever the time course of the signal is.

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CP6

Using Maps to Predict Activation Order in Multiphase Rhythms

We consider a network of three heterogeneous coupled units, each described by a planar dynamical system on two timescales, motivated by recent models for respiratory rhythmogenesis. Each unit's intrinsic dynamics supports an active state and an inactive state. We analyze solutions in which the units take turns activating, allowing for any activation order, including multiple activations of two of the units between activations of the third. The analysis proceeds via the derivation of a set of explicit maps between the pairs of slow variables corresponding to the inactive units on each cycle. Evaluation of these maps on a few key curves in their domains can be used to constrain all possible activation orders in a given network and to obtain boundary curves between all regions of initial conditions producing different activation patterns.

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CP6

The Influence of Heart Rate Variability on Alternans Formation in the Heart

Sudden cardiac death is caused by ventricular fibrillation, which is directly linked to an alternation in action potential duration (APD) at the cellular level, i.e. alternans. A common technique for studying the initiation and of alternans is the restitution curve, i.e. the relationship between the APD and the preceding diastolic interval. However, this technique was derived under periodic pacing condition, i.e. in the presence of feedback. However, in the heart, more complex stimulation regimes exist, including physiological heart rate variability (HRV). Here, we investigated the effect of HRV on the alternans formation in the heart, both at the cellular and whole heart levels.

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CP7

Estimation of 3D Microstructural Band Properties in Dual Phase Steel Assuming An Oriented Cylinder Model

Oriented cylinders in an opaque medium represent microstructural banding in steels. The medium is sliced and on the cut plane, rectangular projections of the cylinders are observed. The marginal distributions of the cylinder radii and heights, aspect ratio, surface area and volume are estimated from the rectangle length and height distributions. This estimation procedure is used on real banded microstructures for which nearly 90 μm of depth have been observed via serial sectioning.

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CP7

Thermodynamically Compatible Model of Yield Stress Polymeric Fluids

We want to present some results on mathematical modeling of polymeric yield stress fluids which have the properties of both elastic solids and fluids. We try to investigate this problem using the approach of multiphase continuum mechanics. We develop the two-phase solid-fluid model which is thermodynamically compatible and its governing differential equations can be written in a conservative form. Such a model is convenient for application of advanced high-accuracy numerical methods and modeling of discontinuous solutions.

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CP7

Temporal Coarse-Graining of High Frequency Dynamics Using Parameterized Locally Invariant Manifolds

A model is built for coarse representation of the dynamics of phase transitions at the atomistic level. The coarse model is based on the idea of Parameterized Locally Invariant Manifolds (PLIM). By considering fine dynamics as a system of ODE, one generates an evolutionary set of closed equations for the coarse quantities. With the implementation of PLIM, we observe the macroscopic features of the system, such as temperature, number of interfaces and the stress-strain curve.

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CP7

Dynamics of Light Beam Interaction at the Interface of Nonlinear Optical Media

The Dynamics of two or more light beams interacting at the interface of linear and nonlinear optical media is studied numerically and analytically. Some interesting new results have been obtained. The numerical Simulations agree with the results of analytical model. This results can be used to develop devices in optical beam switching.

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CP7

Impact of Combined Irregularity on the Torsional Wave Propagation

In this paper, we study the propagation of torsional surface wave in a homogeneous layer over an initially stressed heterogeneous half space with linearly varying directional rigidities, density and initial stress under the effect of various combined irregularities at the interface. Dispersion equation in a closed form has been deduced for various cases. For a layer over a homogeneous half space, the velocity of torsional surface wave coincides with that of the Love waves. The consolidated effect of combined irregularity, inhomogeneity, initial stress and wave number on the phase velocity of torsional wave is depicted by means of graphs.

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CP8

Matrices, Kirchhoff Graphs and Reaction Networks

This talk introduces the concept of a Kirchhoff graph for any rational matrix. Kirchhoff graphs represent the fundamental theorem of linear algebra for the matrix; if the matrix is the stoichiometric matrix for a chemical reaction networks, they also satisfy the Kirchhoff laws for that reaction network. The construction of these graphs and some of their properties will be discussed.

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CP8

Microscopic Theory of Brownian Motion Revisited

A single massive particle suspended in a non-interacting solvent is studied. Microscopic expressions for the friction coefficient in the Langevin equation in the Brownian limit and the time autocorrelation function of the force on the Brownian particle in the frozen dynamics are presented. Guided by these expressions, the limiting behaviors of Mori kernel, which is numerically obtained from molecular dynamics simulation results of the full dynamics, are observed and discussed.

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CP8

A Conjecture on the Structure of Mutually Unbiased Bases

The maximal size of a collection of mutually unbiased bases (MUBs) for a finite-dimensional, complex Hilbert space is only known for certain dimensions. We offer a conjecture concerning the structure of the space of MUBs and prove it for dimension 2, which provides a new proof that the maximum size of a collection of MUBs is 3. We also develop a new algorithm for generating random MUBs to numerically explore conjectures concerning MUBs.

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CP8

Recursive Fermi-Dirac Operator Expansions with Applications in Electronic Structure Theory

Recursive Fermi-Dirac operator expansion is an efficient way to calculate the density matrix in reduced complexity electronic structure theory. In this work, the errors in the recursive expansion methods are analyzed and schemes for error control developed. Besides error control, a scale-and-fold technique to accelerate the convergence of the recursive expansion for the zero temperature case will be presented.

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CP8

Block-Sparse Matrix-Matrix Multiplication with Error Control for Quantum Chemistry Applications

In quantum chemistry applications such as Hartree-Fock (HF) and Kohn-Sham density functional theory (KS-DFT) for large molecules, the structure of the involved matrices is such that a sparse matrix representation is advantageous. Efficient matrix-matrix multiplication for such matrices is needed in the computationally challenging density matrix construction operation. In this work, methods for matrix-matrix multiplication for this kind of matrices are developed and evaluated, focusing on efficiency and error control.

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CP9

Time Reversed Absorbing Condition (trac): Applications to Inverse Problems

We introduce time reversed absorbing conditions (TRAC) in time reversal methods. They enable one to "recreate the past' without knowing the source which has emitted the signals that are back-propagated. Applications in inverse problems are presented. The method does not rely on any a priori knowledge of the physical properties of the inclusion. Numerical tests with the wave equation illustrate the efficiency of the method. This technique is fairly insensitive with respect to noise in the data.

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CP9

Reducing Uncertainty in Stochastic Inverse Problems Involving Sparse Data

This work presents an approach for augmenting the information in the posterior distribution accompanying Bayesian inverse problems. Dominant behavioral features of a particular system, captured using snapshots from a physics based model, in conjunction with a "Gappy' inner product are used to generate plausible surrogate data. Such data are incorporated into the likelihood function to reduce the uncertainty in the joint posterior over model parameters. Numerical examples are provided for characterization and flaw identification.

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CP9

An Application of Particle Swarm Optimization to Identify the Thermal Properties of Materials

Input your abstract, including TeX commands, here. The abstract should be no longer than 75 words. Only input the abstract text. Don't include title or author information here. An inverse analysis of identifying thermal properties for materials is presented. It is shown that the physical problem can be formulated as an optimization problem with differential equation constraints. A particle swarm optimization algorithm is developed for solving the resulting optimization problem. The proposed algorithm provides a global optimum with highly-improved convergence performance. Numerical results are presented to demonstrate the performance of the proposed method. The comparison to the modified genetic algorithm is also included.

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CP9

The Estimation of Uncertainty in the Solution of Ice Sheet Inverse Problems: Gaussian Linear Case versus the Stochastic Newton MCMC Method

We consider the estimation of uncertainty in the solution of ice sheet inverse problems within the framework of Bayesian inference. When the noise and prior probability densities are Gaussian, and the parameter-to-observable map is linearized, the resulting posterior probability density is Gaussian, with covariance given by the inverse of the log-posterior Hessian. We compare solutions of ice sheet inverse problems under the Gaussian-linear assumption with the full non-Gaussian solution obtained by stochastic Newton MCMC sampling, which employs local Hessian-based Gaussians as proposal densities.

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CP9

A Comparison of Deterministic and Stochastic Means for Damage Parameter Identification in a Multiphysics Context

A means for obtaining accurate damage parameter estimates resulting from complex, multi-modal likelihood functions common with multiphysics problems is presented. Noisy data in the form of fluid pressures resulting from the vibration of a damaged structure are generated from sparse sensors in the fluid domain. A comparison between a deterministic and stochastic means for solving the inverse problem is described. Solution existence, uniqueness and stability will be discussed.

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CP9

3-D Constrained Joint Inversion of Geophysical Data for Crustal and Mantle Velocities in the Southern Rio Grande Rift

We propose a novel approach for joint inversion of geophysical datasets to characterize velocity structure of the Rio Grande Rift. The inverse problem is solved as in nonlinear programming with interior-point methods. We introduce physical bounds over the model parameters and a measure of differences in geological structure. Bound and structural constraints introduce a priori information to simulate the physics of each dataset. Initial results reveal 3-D velocity structure suggesting continuation of deformation and

extension of the Rift.

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CP10

Modeling and Analysis of Plant-Seed Bank Dynamics of a Disturbance Specialist in a Random Environment

A nonlinear stochastic integral projection model (SIPM) is introduced for the dynamics of a plant population with a seed bank. This plant population needs disturbances to germinate, and these disturbances are governed by a stochastic process. Under biologically-reasonable assumptions we show that both the plant and the seed bank populations converge (in distribution)to a stationary distribution independent of initial populations. We also show how changes in the parameters governing disturbance (frequency and intensity of disturbance)affect some of the characteristics of the long-term stationary distribution.

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CP10

Urinary Tract Infections in Meningioma Patients: Analysis of Risk Factors and Outcomes

Urinary tract infections account for approximately 35% of all nosocomial infections and 75% are associated with the use of urethral catheters. The goal of this study was to evaluate pre-operative factors associated with the risk of a UTI and estimate the impact of UTIs on patient outcome and resource utilization. Perioperative UTIs were strongly associated with specific comorbidities and post-operative complications. They significantly increase in-hospital length of stay and costs.

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CP10

Finding Trends in Multiscale/Non-Stationary Time Series

We would like to define a trend to a a time series for which there is no information on its statistics or for which an approximate or a precise functional relationship to time is not known or safely assumed. An example where this arises is in the determination of whether meteorological variations can be ascribed to simple fluctuations, or are instead manifestations of changes in the global climate trend. We introduce an adaptive non-parametric time series estimator that has a clear mathematical description and is capable of extracting a trend for this type of time series.

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CP10

Linear Regression Via the Singular Value Decomposition

Biased estimators for linear ill-posed problems are often obtained by truncating the SVD for the discrete system. The technique is generally regarded as a determination of the "numerical rank" of the matrix, even though this "rank" often depends on the right hand side vector. A better idea is to truncate the rotated right hand side vector to eliminate components corrupted by measurement errors. The method also works well for well conditioned regression problems.

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CP10

Large Deviations and Importance Sampling for a Feed-forward Network

We begin by considering a feed-forward network with a single server station serving jobs with multiple levels of priority. The service discipline is preemptive in that the server always serves a job with the current highest priority level. For this system with discontinuous dynamics, we outline that the family of scaled state processes satisfy the sample path large deviations principle using a weak convergence argument. In the special case where the jobs have two different levels of priority, we explicitly identify the exponential decay rate of the probability a rare event, namely, the total population overflow associated to the feed-forward network. We then use importance sampling - a variance reduction technique - efficient for rare event probabilities to simulate the exact probability of interest. We conclude by confirming our theoretical results with numerical simulations.

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CP10

Demonic Fuzzy Operators: Illustration with Fuzzy Logic

Fuzzy relations and fuzzy relational operators can be used to define the fuzzy semantics of programming languages. The operators $\cup_{fuz}$ and $\circ_{fuz}$ serve to give an *fuzzy angelic semantics*, by defining a program to go right when there is a possibility to go right. On the other hand, the fuzzy demonic operators $\sqcup_{fuz}$ and $_{fuz}$ do the opposite: if there is a possibility to go wrong, a program whose semantics is given by these operators will go wrong; it's the *fuzzy demonic semantics*. We will define these operators and illustrate them using fuzzy logic.

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CP11

Fast Computation of the Zeros of a Polynomial

We present a new method for computing the zeros of a polynomial based on a factorization of the companion matrix into a product of $n-1$ essentially 2×2 matrices. The zeros are computed by a non-unitary variant of Francis' algorithm that preserves the matrix factorization and consequently uses only $O(n)$ storage and produces the roots in $O(n^2)$ time.

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CP11

A One-Sided Convex Area Function for Improved Variational Grid Generation

The use of suitable convex area functionals in the context of the variational grid generation problem has been studied in detail. A fundamental theorem for this problem states that if Ω is a polygonal region for which there exists a convex grid, and $f : \mathbf{R} \to \mathbf{R}$ is a C^2 convex, strictly decreasing and nonnegative function, then it is possible to find a real number t such that the functional $F : \mathbf{R^N} \to \mathbf{R}$ given by $F(G) = \sum_{q=1}^{N} f(t\alpha_q)$ attains its minima in the open set of convex grids for Ω. Using this result, several global and local strategies for updating t have been proposed. In this paper, by weakening the strictly decreasing hypothesis, we propose a one-sided functional, for which $f(x)$ is constant for x larger that a given parameter α_0. This new functional is also convex and shares many properties with the previous ones, but since it focuses only on grid cells with area values less that α_0, it can be used in order to increase the quality of very specific cells on convex grids. Some numerical experiments show the quality grids that can be obtained with this new approach.

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CP11

A Scalable Reformulation of the Parallel Algorithm for the Mixed Volume Computation

Efficient algorithms for computing mixed volumes have been implemented in DEMiCs and MixedVol-2.0. While the approaches in those two packages are different, they follow the same theme and are both highly serial. To fit the need for the parallel computing, a reformulation of the algorithms is inevitable. In this talk, a reformulation of the algorithm for the mixed volume computation rooted from algorithms in graph theory will be presented.

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CP11

Accelerating Iterative Linear Solvers on GPU

In this talk we present new results on developing parallel iterative linear solvers on NVIDIA GPU. We have designed a new matrix vector multiplication kernel and other BLAS 1/2 subroutines. Based on these subroutines, seven Krylov solvers and two algebraic multigrid solvers were implemented. ILU(k), ILUT, approximate inverse, polynomial, domain decomposition and algebraic multigrid preconditioners were also developed. Besides, a parallel triangular solver was developed. The speedup of our solvers was up to 20.

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CP11

Nonoverlapping Domain Decomposition Preconditioners for Isogeometric Analysis

In this talk, we construct and study nonoverlapping domain decomposition preconditioners for elliptic problems discretized by NURBS-based Isogeometric Analysis. We consider nonoverlapping preconditioners for the reduced Schur complement system, in particular BDDC preconditioners defined by primal continuity constraints across the subdomain interface. These constraints are associated to subdomain vertices and/or averages or moments over edges or faces of the subdomains, but have a higher multiplicity proportional to the splines regularity. By constructing appropriate discrete norms, we are able to prove that our isogeometric BDDC preconditioner is scalable in the number of subdomains and quasi-optimal in the ratio of subdomain and element sizes. Numerical experiments in 2D and 3D that confirm our theoretical estimates and also illustrate the preconditioner performance with respect to the polynomial degree and regularity of the NURBS basis functions, as well as its robustness with respect to discontinuities of the elliptic coefficients across subdomain boundaries.

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CP11

Dynamic Implicit 3D Adaptive Mesh Refinement For Non-Equilibrium Radiation Diffusion

We describe a highly effifficient solution method for the coupled nonlinear time dependent non-equilibrium radiation diffffusion equations. This coupled system of nonlinear equations exhibits multiple temporal and spatial scales rendering it a stiffff coupled system to solve. Fully implicit time integration schemes are combined with 3D parallel adaptive mesh refinement with the resulting nonlinear systems at each timestep being solved with a Jacobian Free Newton Krylov method which employs highly efficient physics based multilevel preconditioners.

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CP11

Recursive Schur Decomposition

We will present a new preconditioner to solve the linear systems of equations arising from the discretization of elliptic partial differential equations (PDEs) using the finite element method. This is a recursive algorithm that uses (a) non-overlapping domain decomposition, (b) Schur decomposition, (c) Krylov subspace method and (d) a fast solver such as multigrid. We will also describe the parallel implementation of this algorithm. Although the algorithm is general enough to be applied to solve a wide variety of elliptic PDEs, we will focus on a model Poisson problem for demonstration purposes. The algorithm can also be extended to other discretizations such as finite difference or finite volume methods.

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CP12

Schur Complements and Block Preconditioners for Coupled Diffusion Systems

Discretization of systems of coupled PDE under finite elements or finite differences gives rise to block-structured algebraic systems. Expensive to solve, these systems require effective preconditioning. Many of these preconditioners are based on block LU factorizations. In such factorizations, one obtains the Schur complement by eliminating one field in terms of the other. Preconditioners constructed in this manner require the inverse of the Schur complement, which is very expensive to compute. We study a particular simple strategy for approximating the Schur complement that has some general applicability, giving examples both of the resulting block preconditioner and solving the Schur complement system for some coupled PDE.

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CP12

Absolutely Stable Explicit Difference Schemes Possessing Unconditional Approximation. Parabolic Equation Case.

A difference scheme is proposed that is absolutely stable as implicit schemes and require the minimum number of arithmetic operations as explicit schemes. It also proposes a version of the Du Fort - Frankel scheme possessing unconditional approximation.

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CP12

Instability of the Finite-Difference Split-Step Method on a Non-Constant-Amplitude Background in the Nonlinear Schrödinger Equation (nls)

We consider the implementation of the split-step method where the linear part of the NLS is solved by the Crank-Nicolson method employing finite-difference discretization of the spatial derivative. The von Neumann analysis reveals that this method is unconditionally stable on the background of a constant-amplitude plain wave. However, simulations show that the method can become unstable on the background of a *soliton*. We present a theory explaining this instability. Both this theory and the instability itself are substantially different from those of the Fourier split-step method, which computes the spatial derivative by spectral discretization.

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CP12

Using the Reverse Heat Equation to Approximate Fields Using Gaussian Basis Functions

Field interpolation is any method for approximating a known field as a linear combination of basis functions. This presentation explores a procedure using the reverse heat equation to produce high order representations of the known field. As an alternative to interpolation methods, we will begin with a regularization of the known field and use direct, stable, explicit finite difference methods to correct the regularization using the reverse heat equation. This method achieves the predicted second, fourth and sixth order of accuracy.

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CP12

Uniform Numerical Approximation of Integrable Equations via Riemann-Hilbert Problems

The Riemann–Hilbert formulations of the Korteweg–de Vries and the Painlevé II transcendent have proved to be computationally valuable. Borrowing ideas from the method of nonlinear steepest descent, the resulting numerical schemes are seen to be asymptotically reliable. Here we derive some sufficient conditions for a numerical method to maintain accuracy throughout unbounded regions of the plane on which the differential equation is posed.

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CP12

On the Numerical Solution of Initial-Boundary Problem to One Nonlinear Parabolic Equation

In the presented work the numerical solution of initial-boundary problem to the following nonlinear parabolic equation

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

is obtained. The coefficients $a\,(x,\,t,\,U)$ and $b\,(x,\,t,\,U)$ are required to be continuous and to have continuous partial derivative with respect to argument U. Additionally coefficient $a\,(x,\,t,\,U)$ is required to be positive. The function $f\,(x,\,t)$ is required to be continuous. For the mentioned initial-boundary problem the difference scheme is constructed and the theorem of existence of its solution and the theorem of convergence of its solution to the solution of the source problem are proved. The rate of convergence is established and it is equal to $O\left(\tau + h^2\right)$.

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CP12

Investigations on Performances of Electromagnetic Solvers

Many efficient numerical methods have been developed and used for electromagnetic simulations in time and frequency domains. Their performances are quite different based on many details of the numerical methods, such as mesh, numerical orders and expansion bases, etc. This talk will investigate these factors and compare their performance in detail. Some simulation results will be presented using the suitable solvers. Challenges for current solvers and possible new techniques to improve them will be discussed.

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CP13

Data Mining Methods Applied to Numerical Approximations for Pdes

Classical results analysis of numerical methods is very often limited to the description of tables or graphs of isovalues. We propose a new method for numerical data analysis, based on exploratory data mining techniques that have proven to be efficient in other areas producing bulimic data, like biology or marketing. Our approach allows us to analyze and characterize the different sources of errors involved in a given mathematical modeling process coupled with numerical approximations.

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CP13

Runge-Kutta Discontinuous Galerkin Method for 2D Nonlinear Moment Closures for Radiative Transfer

Radiative transport equation calculations have important applications in determining the interaction between high energy particle propagation and body tissue in radiation dose therapy. We apply the Runge-Kutta discontinuous Galerkin (RKDG) method to moment models for the radiative transfer equation. Our goal is to resolve the time evolution of isolated sources or beams of particles in heterogeneous media on unstructured grids. The moment models considered are nonlinear hyperbolic balance laws.

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CP13

The Ghost Solid Method Based Algorithms for Elastic Solid-Solid Interaction

Three variations of Ghost Solid Method based algorithms are developed for capturing the boundary conditions at the solid-solid interface of isotropic, linearly elastic materials, in a Lagrangian framework. The methods are extensively tested under 1D setting. The effect of using different solvers for these methods is discussed. The advantages and disadvantages of each of these methods are analyzed. Preliminary results show that these methods can be extended to multi-dimensional settings.

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CP13

Applying the Exterior Matrix Method to the Inclined Cable Problem

We apply the Exterior Matrix Method to find the approximate eigenfrequencies for serially connected inclined cables. The dynamics of each satisfies a system of four partial differential equations, but even their linearization cannot be solved in closed form. However, the Exterior Matrix Method does not require the solution of governing equations. The eigenfrequency information is embedded in a 6×6 exterior matrix for each span, which are multiplied together to solve for the eigenfrequencies.

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CP13

Introduction to the Exterior Matrix Method

We will introduce the Exterior Matrix Method (EMM) to compute the approximate eigenfrequencies for serially connected elements, each governed by a system of four first order linear partial differential equations. Ironically, the governing equations do not have to be solved to find the approximate corresponding 6×6 exterior matrix. We can solve the the approximate eigenfrequencies by multiplying the exterior matrices together. The procedure works even if dissipative joints are added to the system.

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CP13

Highly Accurate Algorithm for Time-Dependent Pde's

Standard space discretization of time-dependant pde's usually results in system of ode's of the form

$$u_t - Gu = s \tag{3}$$

where G is a linear operator (matrix) and u is a time-dependent solution vector. Highly accurate methods, based on polynomial approximation of a modified exponential evolution operator, had been developed already for this type of problems where G and s are constant. In this talk we will discribe a new algorithm for the more general case where G and s depend on t and u. Numerical results will be presented.

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CP14

Small Deformation Viscoplastic Dynamic Sphere Problem

Developing benchmark solutions for problems in solid mechanics is very important for the purpose of verifying computational physics codes. In order to test some physics codes, we present a benchmark solution to the small deformation dynamic sphere problem for an isotropic viscoplastic material obeying the Bodner-Partom model. The solution takes the form of an infinite series of eigenfunctions. We demonstrate convergence under eigenmode, spatial, and time refinement, and then compare to numerical results.

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CP14

Tensor Product Decomposition Methods for Noise Reduction, Data Compression, and Projective Integration

Tensor product decomposition (TPD) methods are a powerful linear algebra technique for the efficient representation of high dimensional data sets. In the simplest 2-D case, TPD reduces to the well-known singular value decomposition of matrices. We discuss the application of TPD methods to data compression of 3-D Magnetohydrodynamic and 6-D kinetic simulations of plasmas. We also discuss the application of TPD methods in noise reduction and projective integration of particle-based collisional transport computations.

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CP14

Lime: Software for Robust and Flexible Multiphysics Coupling

Multiphysics code coupling aims at a synergistic union of existing and emerging simulation capabilities with robust and efficient coupling algorithms. Originally targeting nuclear reactor performance modeling, LIME represents a general multiphysics coupling capability. LIME's algorithms span fixed-point coupling, placing no restrictions on models or methods, through Newton-based coupling, requiring residuals and exploiting any additional information and functionality codes expose. A rich suite of linear and nonlinear solvers is provided through LIME's interface to the Trilinos Solver Framework.

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CP14

Application of a Perturbation Method to Nonlinear Parabolic Stochastic PDEs

We have applied the perturbation method developed by Zhang and Lu in 2004, making use of the Karhunen-Loève expansion, to 2D parabolic equations having stochastic conductivity and nonlinear reaction. Some results are shown, demonstrating that in many cases the method produces good approximations of the first and second moments of solutions. Some analysis of computational complexity and convergence of the approximate solutions will be presented.

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CP14

Discontinuous Galerkin Methods for Modelling and Simulation of Transcription Processes

A Discontinuous Galerkin FEM is used for simulation of a nonlinear PDE that models the motion of polymerases on ribosomal RNA. Physically relevant pauses along the rrn operon are incorporated into the model. These pauses result in delays during the transcription process, possibly affecting protein production. The average delay experienced by a polymerase is estimated, and sensitivity analysis is used to quantify the effects that location and time duration of pauses have on the average delay.

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CP14

Reweighted l_1 Minimization Method for SPDEs

We propose a method for the approximation of solutions of PDEs with stochastic coefficients and "sparse" solutions based on l_1 minimization. We employ reweighted iterations to enhance the "sparsity" of the solution. Also, we use sampling points based on specific probability measure due to the structure of the measurement matrix which depends on the gPC expansion of the solutions. This non-intrusive method is especially effective when the deterministic solver is very time consuming.

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CP15

Identity Issues in Radial Basis Functions: RBFs As Modulated Sinc Functions in the Near-Equivalence of Exponentially Convergent RBF Species

On a one-dimensional uniform, infinite grid, we show that radial basis functions (RBFs) are well approximated by the product of the sinc, $\sin(\pi x)/(\pi x)$, with a modulation $\pi x/\sinh(\pi x/\rho)$. This implies that Gaussian, sech, multiquadric, inverse multiquadric and inverse quadratic RBFs are the same species,modulo tiny differences that disappear altogether in the "flat limit". Extensions to a nearly uniform grid and to higher dimensions are also described..

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CP15

Error Bounds for Spline Interpolation Based Parametric Model Order Reduction

Spline interpolation technique combined with balanced truncation is con- sidered to reduce the order of parameter dependent large LTI-systems while preserving the parameters as variables. Linear or cubic spline inter- polation is applied to transfer functions of locally reduced order models to deliver an approximation to the parameter dependent original transfer function. This talk presents the procedures and the derivation of error bounds and demonstrates the results on a numerical example.

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CP15

Chebyshev Interpolation for Functions with End-

point Singularities.

Functions defined on a finite interval which are bounded and singular at one or both endpoints may be effectively dealt with by use of an exponential or double-exponential transform. This strategy involves transplantation of the problem function to an infinite or semi-infinite interval, where a trade-off between domain-truncation and interpolation errors determines the overall rate of convergence. We shall systematically categorise the convergence theory for these situations, with a particular focus on Chebyshev interpolation.

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CP15

Finite Difference Weights and Superconvergence

Let $z_1, z_2, \ldots, z_N$ be a sequence of distinct grid points. A finite difference formula approximates the m-th derivative $f^{(m)}(0)$ as $\sum w_k f(z_k)$. We derive an algorithm for finding w_k which uses fewer arithmetic operations and less memory than the algorithm in current use (Fornberg, Mathematics of Computation, vol. 51 (1988), p. 699-706). In addition, the order of accuracy of the finite difference formula for $f^{(m)}(0)$ with grid points $hz_k, 1 \le k \le N$, is typically $\mathcal{O}\left(\langle^{\mathcal{N}-\Updownarrow}\right)$. However, the most commonly used finite difference formulas have an increased order of accuracy (superconvergence). Even unsymmetric finite difference formulas can exhibit such superconvergence, as shown by the explicit algebraic condition that we derive.

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CP15

Jacobi 1825, Cauchy 1826, Poisson 1827

Fast-converging numerical algorithms are usually fast because some function is analytic, and to quantify that fast convergence, a powerful tool is contour integrals in the complex plane. We show how a formula in Jacobi's 1825 thesis in Berlin leads to:

- fast convergence of the periodic trapezoid rule
- Hermite integral formula
- Runge phenomenon
- potential theory
- Euler-Maclaurin formula
- Gauss quadrature
- spectral methods
- barycentric interpolation formula
- Chebfun
- (and maybe) hyperfunctions

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CP15

Barycentric Hermite Interpolation

For long it was believed that Newton interpolation was superior to Lagrange interpolation. However, the work of Berrut and Trefethen has shown that Lagrange interpolation is as fast and typically more robust. Here we consider Hermite interpolation: finding a polynomial interpolant that matches the function values and derivatives at grid points. We derive an algorithm for barycentric Hermite interpolation. The algorithm is identical to the recently published version of Butcher et al. (Numerical Algorithms 2011). However our derivation is somewhat different and leads to an efficient method for updating Hermite interpolants.

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CP15

Summability of Expansions on the Cylinder

We present a result regarding the Cesàro summability of the expansion of functions on the cylinder $B^d \times I^m$ in orthogonal polynomials with respect to a product weight function. An upper bound for the critical index δ is obtained.

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CP16

Numerical Methods for High-Dimensional Pdf Equations

We study the evolution equation of joint excitation-response PDF obtained by the Hopf functional approach for various stochastic systems. Adaptive Discontinuous Garlerkin and other methods are developed and compared to solve this advection-type evolution equation. Also, some issues arising in this formulation are investigated including different high dimensionality in phase and parametric space, and representation of multiple correlated random processes. Various stochastic dynamical system such as nonlinear advection equation, tumor cell model, and Limit Cycle Oscillator are tested.

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CP16

A Convergence Study for Spdes Using Combined Polynomial Chaos and Dynamically Orthogonal

Schemes

We study the convergence properties of the recently developed Dynamically Orthogonal (DO) field equations in comparison with the Polynomial Chaos (PC) method. A hybrid method with PC is introduced to tackle the singularity of the DO equations for the case of deterministic initial conditions. An adaptive method in the basis is also proposed. The computational cost of DO is found to be smaller when compared to the cost of other methods including MC and PC.

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CP16

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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CP16

Variance-Reduced Equation-Free Newton-Krylov Methods for Stochastic Fine-Scale Simulations

Equation-free methods promise a straightforward computation of macroscopic steady states and their stability, based only on appropriately initialized short bursts of microscopic simulation, which are used to compute residuals and Jacobian-vector products. One way to proceed is to use a Newton algorithm, in which the linear systems in each Newton iteration are solved via a Krylov method. A major problem in a naive implementation of this approach is the amplification of statistical noise in the Jacobian-vector products when the microscopic model is stochastic. This talk discusses approaches to reduce the variance on these Jacobian-vector calculations significantly, yielding significant reductions in computational effort.

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CP16

Stochastic Collocation Methods for Stochastic Differential Equations Driven by White Noise

We propose stochastic collocation methods for SODEs and SPDEs driven by white noise using the Stratonovich formulation. To control the increasing dimensionality in random space generated by the increments of Brownian motion, we approximate Brownian motion with a spectral expansion. We also use sparse grid techniques to further reduce the computational cost. Numerical examples demonstrate the very high accuracy and efficiency of the proposed method, including equations driven by additive and multiplicative noises.

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CP17

Multigrid, Adaptive Discontinuous Galerkin Methods for the Cahn-Hilliard Equation and a Diffuse Interface Model of Tumor Growth

We present a mixed discontinuous galerkin finite element (DG-FE), convex splitting scheme for the Cahn-Hilliard (CH) equation. Unconditional energy stability and unique solvability, as well as optimal convergence, are proven for the scheme. An efficient non linear multigrid algorithm is used to solve the discrete equations. Also, a spatially adaptive, primitive-variable DG-FE scheme for a CH-type diffuse interface model for cancer growth is presented. Convergence under mesh modification is demonstrated, and simulation results are provided.

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CP17

An Efficient Scheme Involving Only Constant Coefficient Matrices for Coupled Navier-Stokes/Cahn-Hilliard Equations with Large Density Ratios

We present an efficient scheme for simulations of the coupled Navier-Stokes/Cahn-Hilliard equations for the phase field approach. The scheme has several attractive features: (i) It is suitable for large density ratios, and numerical experiments with density ratios up to 1000 have been presented; (ii) It involves only time-independent coefficient matrices for all flow variables, which can be pre-computed during pre-processing, so it effectively overcomes the performance bottleneck induced by variable coefficient matrices associated with the variable density and variable viscosity; (iii) It completely de-couples the computations of the velocity, pressure, and the phase field function. Simulations will be presented to demonstrate the effectiveness of current method for studying two-phase flows involving large density ratios, moving contact lines, and interfacial topology changes.

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CP17

Application of Compact-Reconstruction WENO Schemes to the Navier-Stokes Equations

The Compact-Reconstruction WENO (CRWENO) scheme was constructed by applying the WENO algorithm on compact stencils and achieved high spectral resolution as well as non-oscillatory behavior across discontinuities. The new scheme was analyzed for scalar conservation laws and the Euler equations. The CRWENO scheme demonstrated lower dissipation and dispersion errors for smooth and discontinuous flows, compared to the WENO scheme. In the present study, the CRWENO scheme is applied to the multi-dimensional Navier-Stokes equations on curvilinear meshes. Results are presented for steady flow over airfoils as well as dynamic stall of a pitching airfoil. Flow problems representative of direct numerical simulation (DNS) of turbulent flows are attempted and the results from the CRWENO scheme are compared with those from the WENO scheme.

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CP17

A Fast Perturbation Approach in Ensemble Level Upscaling

Ensemble level upscaling is efficient upscaling of flow parameters for multiple geological realizations. Solving the flow problem for all the realizations is time-consuming. Recently, different stochastic procedures have been combined with upscaling methods to efficiently compute the upscaled coefficients for a large set of realization. In this work, we proposed a fast perturbation approach in the ensemble level upscaling. We give a correction scheme to generate upscaled parameters and use collocation and clustering techniques in stochastic space, which allow us to compute the upscaled permeabilities rapidly for all realizations. The numerical results will be present.

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CP17

Summation-by-Parts Operators and Weak Initial Conditions for Time-Discretisation

During the last decade, stable high order finite difference methods applied to initial-boundary-value-problems have been developed. The stability is due to the use of so-called summation-by-parts operators (SBP), penalty techniques for implementing boundary and interface conditions (SAT), and the energy method for proving stability. The so called SBP-SAT technique has so far only been used to discretize the initial-boundary-value-problem in space. In this talk we will discuss the use of this technique also in time. For linear problems, the result will be a fully discrete and energy stable method of very high order of accuracy. We will discuss stability, accuracy and efficiency aspects of this technique.

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CP17

Partitioned Algorithms for the Numerical Solution of the Fluid-Structure Interaction Problem in Haemodynamics

In this work we deal with the numerical solution of the fluid-structure interaction (FSI) problem arising in the haemodynamic environment. The aim is to develop efficient partitioned algorithms for real haemodynamic applications, where the non-linear finite elasticity is considered for the structure subproblem. We provide theoretical and experimental results concerning the accuracy and efficiency of the proposed schemes and finally we apply some of such schemes to the case of human carotid geometries, in order to compare the fluid-dynamics before and after the removal of the atheromasic plaque.

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CP18

Guaranteed Biclustering Via Semidefinite Programming

Given a set of objects and a set of features exhibited by these objects, biclustering seeks to simultaneously group the objects and features according to their expression levels. We pose this problem as that of partitioning a weighted complete bipartite graph such that the densities of the resulting subgraphs are maximized. We consider a nonconvex quadratic programming formulation for this problem and relax to a semidefinite program using matrix lifting. We show that the correct partition of the objects and features can be recovered from the optimal solution of the semidefinite relaxation in the case that the input instance consists of several disjoint sets of objects exhibiting similar features.

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CP18

A Minty Variational Principle for Set-Valued Optimization

Set-valued optimization is proving a valuable tool in mathematical finance (see e.g. F.Heyde et al. in Math.Meth.Oper.Res (2009) 69:159-179). Besides, in scalar and vector optimization, Minty variational principle proves to be a sufficient optimality conditions and ensures good properties of the primitive optimization problem. We want to develop a Minty variational principle for set-valued optimization, defining Dini-type derivative for set-valued functions.

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CP18

Solving Games by Differential Equations in Finite Time

New method to solve symmetric matrix games by differential equations is described. It allows us to find out optimal mixed strategy in finite time, whilst the ODE-based method, belonging to Brown and von Neumann, in general case consideres ODE on $[0, \infty)$ and gives only the value of game.

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CP18

Solving Sup-$\mathcal{T}$ Equation Constrained Optimization Problems

This work considers solving the sup-$\mathcal{T}$ equation constrained optimization problems from the integer programming viewpoint. A set covering-based surrogate approach is proposed to solve the sup-$\mathcal{T}$ equation constrained optimization problem with a separable and monotone objective function in each of the variables. This is our first trial of developing integer programming-based techniques to solve sup-$\mathcal{T}$ equation constrained optimization problems. Our computational results confirm the efficiency of the proposed method and show its potential for solving large scale sup-$\mathcal{T}$ equation constrained optimization problems.

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CP18

A Joint Economic Production and Delivery Quantity Model With a General Transportation Cost Structure

A joint economic production and delivery quantity model in a delivery price-based supply chain is studied in this paper. More specifically, a fixed lot sizing policy is implemented in the production system, while smaller shipping quantity with periodic dispatches is delivered to the customer. The considered cost includes setup cost to launch the batch production, inventory carrying cost, and transportation cost, where the transportation cost is a general function of the delivery quantity. A per unit time cost model is developed and analyzed to determine the optimal production quantity for the production system and the delivery quantity to the customer. Under some mild conditions, it can be shown that the joint cost function is convex and the optimal production quantity is dependent of the delivery quantity. The computational study has demonstrated the significant impact of the joint decision model on the operating cost. In particular, cost savings can be more than 30% when inventory carrying cost and/or transportation cost are high.

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CP18

Cyber-Insurance in Internet Security: The Problem of Resolving Information Asymmetry

Internet users such as individuals and organizations are subject to different types of epidemic risks such as worms, viruses, spams, and botnets. To reduce the probability of risk, an Internet user generally invests in traditional security mechanisms like anti-virus and anti-spam software, sometimes also known as self-defense mechanisms. However, such software does not completely eliminate risk. Recent works have considered the problem of residual risk elimination by proposing the idea of cyber-insurance. In this regard, an important research problem is resolving information asymmetry issues associated with cyber-insurance contracts. In this paper we propose three mechanisms to resolve information asymmetry in cyber-insurance. Our mechanisms are based on the Principal-

Agent (PA) model in microeconomic theory. We show that (1) optimal cyber-insurance contracts induced by our mechanisms only provide partial coverage to the insureds. This ensures greater self-defense efforts on the part of the latter to protect their computing systems, which in turn increases overall network security, and (2) the level of deductible per network user contract increases in a concave manner with the degree of the user. Our methodology is applicable to any distributed network scenario in which a framework for cyber-insurance can be implemented.

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CP18

Optimal Small Wind Turbine Placement in Constrained Spaces

Wind farms composed of small scale turbines can be economical for small groups interested in renewable energy generation, however the placement of turbines is problematic. There are obstacles, effects of wind shear and wake turbulence that are challenging to address particularly if the available area is limited and there are other constraints. We consider a simple model of these constraints and interference factors and apply steepest descent techniques to optimize turbine placement within constrained spaces.

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CP19

Simulation of Parachute Inflation Using the Front Tracking Method

Front Tracking is a Lagrangian tool for the propagation of material interface and is known for its excellent preservation of interface geometry. We use the front tracking method on a spring system to model the dynamics evolution of parachute canopies. And this mechanical structure is coupled with the incompressible Navier-Stokes solver through the "Impulse Method". We will present the simulation and comparison with experiments of several types of parachute.

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CP19

Drops Settling in Sharp Stratification with and Without Marangoni Effects

We present numerical simulations of a heavy drop settling in a two layer miscible fluid with a sharp stratification in density and surface tension with the drop. When the surface tension is uniform, the drop decelerates significantly as it encounters the lower, denser layer. Intriguingly, when the lower layer has greater surface tension than the upper, the drop may bounce and be prevented from crossing the transition region. In contrast, when the lower layer has lesser surface tension, the drop may accelerate through the transition.

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CP19

A Front-Tracking Method For Moving Fronts And Hyperbolic Conservation Laws

We present a new high-order method for shock capturing with tracked material interfaces. Tracking uses a level set which is advected using the material interface velocity obtained from interfacial Riemann problems. Each material phase is discretized independently using a uniform Cartesian grid and the embedded boundary approach to complex geometry. Our discretization is a high-order Godunov method away from the interface. Near the interface it is a globally conservative and consistent finite volume approach.

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CP19

A Nitsche Method for a Stokes Interface Problem

We present a finite element method for the Stokes equations involving two immiscible incompressible fluids with different viscosities and with surface tension. The interface separating the two fluids does not need to align with the mesh. We propose a Nitsche formulation which allows for discontinuities along the interface with optimal a priori error estimates. A stabilization procedure is included which ensures that the method produces a well conditioned stiffness matrix.

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CP20

Gpu Accelerated Greedy Algorithms for Com-

pressed Sensing

Greedy algorithms for compressed sensing are efficient, suboptimal algorithms to solve the combinatorial optimization problem

$$\min \|x\|_0 \text{ subject to } y = Ax,$$

where $\|\cdot\|_0$ counts the nonzero entries and A is $n \times N$ with $n < N$. Exploiting the computational power of graphics processing units (GPU) permits testing on problems orders of magnitude larger than experiments in the literature. This massive computational acceleration and increase in testing capability provide numerous insights to the greedy algorithms including when each algorithm boasts the best performance.

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CP20

Sparse Support Vector Machines for Classification on Grassmannians

We propose an approach for classifying subspaces, e.g. points on a Grassmannian embedded in Euclidean space, using sparse support vector machines (SSVMs). We consider a labeled set of matrices, either two-class or multiclass, and map these to points on a parameter space. The resulting manifold is embedded in Euclidean space where the SSVM is applied. We present applications to both hyperspectral and medical data sets.

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CP20

Perceptual Grouping of Characters in Antarctica Maps

Our aim is to create a database with information about the name and location of the major geographical features in maps using perceptual grouping. The first step is to segment the characters in names from the background. The centroids of these characters are grouped based on their proximity and direction to other centroids. Our initial tests with simulated text accurately grouped these characters greater than 90% of the time.

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CP20

A Multiobjective Mesh Optimization Framework for Mesh Quality Improvement and Mesh Untangling

We propose a multiobjective mesh optimization framework for mesh quality improvement and mesh untangling. Our framework is able to simultaneously optimize various aspects of the mesh such as the element shape, element size, and associated PDE interpolation error; and to untangle inverted elements, but is not limited to these categories. We successfully apply methods within our framework to real-world applications, such as problems from hydrocephalus and shape optimization.

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CP20

Optical Flow Computations for Solar Irradiance Prediction

We describe our method of short-term solar irradiance forecasting. The method is based on prediction of cloud evolution via optical flow computations from NASA/NOAA satellite imagery. The future cloud configuration is determined and input to Locus Energy's irradiance estimation model to predict irradiance. Our forecasting model was calibrated and validated against NOAA's Surface Radiation network observations; we then further enhance our prediction accuracy by leveraging data from PV installations and weather sensors monitored by Locus Energy.

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CP20

Adaptive Outlier Pursuit in 1-Bit Compressive Sensing and Matrix Completion

In compressive sensing (CS), the goal is to recover signals at reduced sample rate compared to the classic Shannon-Nyquist rate. However, the classic CS theory assumes the measurements to be real-valued and have infinite bit precision. The quantization of CS measurements has been studied recently and it has been shown that accurate and stable signal acquisition is possible even when each measurement is quantized to only one single bit. There are many algorithms proposed for 1-bit compressive sensing and they work well when there is no noise in the measurements, while the performance is worsened when there are a lot of sign flips. We propose a robust method for recovering signals from 1-bit measurements using adaptive outlier pursuit (AOP). This method will detect the positions where sign flips happen and recover the signals using "correct' measurements. Numerical experiments show the accuracy of sign flips detection and high performance of signal recovery for our algorithms compared with other algorithms. This AOP technique can also be applied to solve matrix completion problem when the data is damaged by impulse noise.

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CP21

Effect of Permeability Anisotropy on Density-Driven Flow for CO_2 Sequestration in Saline Aquifers

We present a comprehensive study of the effect of permeability anisotropy on the onset and subsequent development of convection for CO_2 sequestration in saline aquifers. Our linear stability analysis shows that anisotropy reduces the critical time t_C and the critical wavelength λ_C because it amplifies all perturbation modes via an exponential growth factor that is biased towards shorter wavelength modes. Anisotropy increases parity among the modes in such a way that λ_C becomes less meaningful. We have also studied the behavior after t_C using detailed numerical simulations. We show that anisotropy can substantially reduce the time at which the enhanced transport from natural convection becomes significant. In addition, it permits higher mean CO_2 dissolution rates to be sustained for longer periods of time. Our results give strong indication that saline aquifers with permeability anisotropy can provide a means for safe and permanent storage of large amounts of CO_2.

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CP21

Universal Stability Properties for Multi-Layer Hele-Shaw Flows and Its Application to Instability Control

With the motivation of understanding the effect of various injection policies currently in practice for chemical enhanced oil recovery, we study linear stability of displacement processes in a Hele-Shaw cell involving injection of an arbitrary number of fluid phases in succession. This work mainly builds upon our earlier study for the three-layer case [P. Daripa, Studies on stability in three-layer Hele-Shaw flows, *Physics of Fluids*, (20), 2008]. Stability results obtained are universal in the sense that they hold regardless of number of displacing fluids. The stability results have been applied here to design injection policies that are considerably less unstable than the pure Saffman-Taylor case. This is a joint work with my postdoc Xueru Ding. The research reported here has been made possible by a grant NPRP 08-777-1-141 from the Qatar National Research Fund (a member of The Qatar Foundation). The statements made herein are solely responsibility of the authors.

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CP21

Internal Gravity Waves and Their Generation

Time-harmonic internal gravity waves are generated in a stratified fluid by oscillating a rigid object. After removing the time dependence, there remains a boundary value problem for a hyperbolic partial differential equation. We solve this problem when the object is a thin horizontal elliptical plate.

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CP21

A Computational Framework for the Solution of Multi-Material Fluid-Structure Interaction Problems with Crack Propagation

We present a high-fidelity computational framework based on the coupling of an embedded boundary method for CFD and XFEM for the coupled solution of nonlinear fluid-structure interaction problems with large deformations and crack propagation. We illustrate this framework, highlight its features, and assess its performance with the three-dimensional simulation of underwater implosions and pipeline explosions for which test data is available.

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CP21

An Efficient Numerical Method for Solving Coupled Systems of Elliptic Interface and Hyperbolic Partial Differential Equations with Applications to Enhanced Oil Recovery

We will present a fast and efficient method for solving a coupled system of elliptic and hyperbolic equations arising in the context of complex chemical flooding of porous media. The problem involves moving boundaries and discontinuous coefficients. The mathematical model we use is based on the Buckley-Leverett model, Darcy velocity and other complex physics arising from chemicals. To be more exact, we use finite volume method to solve the two-dimensional Riemann problem system, use the finite element method to solve the two-dimensional elliptic interface problem, and the level set method is used to move the interface. The results of our numerical experiments will be presented and discussed. This is an ongoing work. The research reported here has been made possible by a grant NPRP 08-777-1-141 from the Qatar National Research Fund (a member of The Qatar Foundation). The statements made herein are solely responsibility of the authors.

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CP22

Supercritical And Subcritical Hopf Bifurcations On the Van Der Pol Nonlinear Differential Equation

The main purpose of this paper is to discuss following objectives with the famous Van Der Pol Nonlinear Differential Equation: (i) Development of general theory and formulae for determining Hopf Bifurcations on any non-linear Differential equations (ii) Existence of Chaos , Limit Cycles , Supercritical and Subcritical Hopf Bifurcations of Van Der Pols Oscillator and their Statistical analysis .

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CP22

Mathematical Analysis of Chikungunya Model With Discrete Delays

The paper presents the basic model for the transmission dynamics of chikungunya. The model, which consists of seven mutually-exclusive compartments representing the humans and vector dynamics, has a locally-asymptotically stable disease-free equilibrium (DFE) whenever the associated reproduction number () is less than unity. The analyses of the model show the existence of the phenomenon of backward bifurcation (where the stable DFE of the model co-exists with a stable endemic equilibrium when the reproduction number of the disease is less than unity). It is shown, that the backward bifurcation phenomenon can be removed by substituting the associated standard incidence function with a mass action incidence. Analysis of the reproduction number of the model shows that, the disease will persist, whenever > 1. Furthermore, an increase in the length of incubation period, increases the chikungunya burden in the community if a certain threshold quantities, denoted by Δ_b and Δ_v are positive. On the other hand, increasing the length of the incubation period can help reduce disease burden if $\Delta_b < 0$ and $\Delta_v < 0$.

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CP22

Connections Between Phantom Traffic Jams, Jamitons, and Congested Traffic Flow

In this presentation, we show that (a) a wide class of "second-order' macroscopic traffic models (e.g. Payne-Whitham, Zhang-Aw-Rascle) possess traveling wave solutions, called "jamitons', that are analogs of detonation waves in reacting gas dynamics; (b) the occurrence of jamitons is equivalent to the instability of uniform traffic flow, i.e. jamitons serve as models for phantom traffic jams; and (c) the large spread of flow rates in congested traffic regimes that is observed in fundamental diagrams can be explained with the simple 1979 Payne-Whitham model.

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CP23

Boundary Trace Inequalities

This talk will describe some simple boundary trace inequalities for Sobolev functions in $W^{1,p}(\Omega)$ with Ω a bounded region in space with Lipschitz boundary $\partial\Omega$ and $p \leq N$. The inequalities are used to provide new bounds on solutions of inhomogeneous Robin boundary value problems.

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CP23

Γ-Convergence of Inhomogeneous Functionals and Applications to Dielectric Breakdown

The asymptotic behavior of inhomogeneous functionals in Orlicz-Sobolev spaces is studied via Γ-convergence. Applications to the study of (first-failure) dielectric breakdown for composites made of two isotropic phases will be discussed. This is joint work with Mihai Mihailescu (University of Craiova, Romania).

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CP23

Well-Posedness for Euler 2D in Non-Smooth Domains

The well-posedness of the Euler system has been of course the matter of many works, but a common point in all the previous studies is that the boundary is at least $C^{1,1}$. In a first part, we will state the existence of global weak solu-

tions of the 2D incompressible Euler equations for a large class of non-smooth open sets. In a second part, we will give the uniqueness if the open set is the interior or the exterior of a simply connected domain, where the boundary has a finite number of corners. The existence part is a work in collaboration with David Gérard-Varet.

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CP23

Traveling Waves of an Angiogenesis Model

In this talk, we will study travel wave solutions for a class of chemotaxis system modeling the initiation of tumor angiogenesis. The challenges of obtaining traveling wave solutions of such chemotaxis models lie in the high dimensionality and the singularity. Hence the routine approaches, such as phase plane analysis, no longer work. In the talk, we shall show these challenges will be overcome by a Hope-Cole tyoe transformation, such that the transformed system can be solved by the routine approaches. The existence, wave speed and stability of traveling wave solutions will be discussed, and open questions will be presented.

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CP23

Lattice Differential Equation Analysis of Schloegls Second Model for Particle Creation and Annihilation

Schloegls stochastic models for autocatalysis on a lattice of dimension d=2 involves: (i) spontaneous annihilation of particles at lattice sites; and (ii) autocatalytic creation of particles at vacant sites. We analyze the dynamics of interfaces between populated and empty regions via discrete reaction-diffusion equations (dRDEs) obtained from approximations to the exact master equations. These dRDE can display propagation failure absent due to fluctuations in the stochastic model. Higher-level approximations elucidate exact behavior with quantitative accuracy.

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CP23

Uniform Estimate for Non-Uniform Elliptic Equations with Discontinuous Coefficients

Uniform estimate for non-uniform elliptic equations with discontinuous coefficients in heterogeneous media is concerned. The heterogeneous media considered here are periodic and they consist of a connected high permeability subregion and a disconnected matrix block sub-region with low permeability. Elliptic equations with diffusion coefficients depending on the permeability of the media have fast diffusion in high permeability sub-region and have slow diffusion in low permeability sub-region, and they are non-uniform elliptic equations. Let ϵ denote the size ratio of the matrix blocks to the whole domain and let the permeability ratio of the matrix block sub-region to the connected high permeability sub-region be of the order ϵ^2. It is proved that the L^p norm of the gradient of the elliptic solutions in the high permeability sub-region are bounded uniformly in ϵ in bounded and unbounded domains. One example also shows that the L^p norm of the gradient of the solutions in the disconnected subset may not be bounded uniformly in ϵ. It is also noted that the L^p norm of the second order derivatives of the elliptic solutions in the high permeability sub-region in general are not bounded uniformly in ϵ.

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MS0

Continuous and Discrete Models for Infectious Diseases

In this talk, I will present a few representative papers that I have coauthored with Carlos Castillo-Chaves and others. These include some of the earlier work on continuous models for TB and influenza and more recent papers on discrete epidemic models.

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MS0

From Rockstar Researcher to Selfless Mentor: An Overview of the Achievements of Carlos Castillo Chavez

Carlos Castillo Chavezs record of scholarship is unparalleled, representing some of the most important contributions in the study of disease dynamics. Yet, it is a commitment to mentoring that has captivated his interest. In this brief overview, I will chart how Carlos Castillo Chavez not only reached the pinnacle of his field, but how he then turned that same dedication to others, becoming one of the most honored mentors in the sciences.

Melissa Castillo-Garsow
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tba

MS0

Modeling and Quantifying the Transmission Dynamics and Control of Infectious Diseases

I will discuss my research experience working under the supervision of Carlos Castillo-Chavez from my participation in the Mathematical and Theoretical Biology Institute's Summer Research Program to my doctoral work at Cornell. In addition, I will provide an overview of some recent collaborative projects with Carlos and others with a particular focus on research on the transmission and control of emerging and re-emerging infectious diseases.

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MS0

Insights Gained from Modeling Epidemics

I will review some of the insights gained from my collaborations with Carlos Castillo-Chavez in creating create new models that can anticipate the spread of a disease and evaluate the effectiveness of different approaches for bringing an epidemic under control. The talk will provide an overview, for general audiences, of what type of insights these models can provide. I will describe some of the mathematical advances needed to create the next generation of models, and share my personal experiences working with Carlos to create models for controlling the spread of HIV/AIDS, SARS, dengue fever, foot and mouth disease, Ebola, and preparing for a bioterrorist attack.

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MS0

Influenza and Other Infectious Diseases

The complicated dynamics of influenza A exhibit fluctuations on multiple scales, due to the interplay of factors such as age structure, cross-reactivity, and seasonal forcing. To address this interplay, Castillo-Chavez and collaborators developed a comprehensive mathematical framework, and analyzed the potential for sustained oscillations. This lecture will review this work, set it in the context of what came before and after, and complement with discussion of some of Carlos's other contributions to mathematical biology.

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MS1

New Directions in Algebraic Coding Theory

Abstract not available at time of publication.

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MS1

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS1

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS1

Deep-LLL Reconsidered

Lattice reduction plays an important role both in coding theory and cryptography. For example, it has broad applications in cryptanalysis. The Deep-LLL lattice reduction algorithm, as an improvement of classical LLL, was not studied very well as it is outperformed by BKZ reduction. We want to argue why the concept of Deep Insertions could improve reduction algorithms like BKZ and provide empirical evidence.

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MS2

Evasion Paths in Mobile Sensor Networks

Imagine that disc-shaped sensors wander in a planar domain. A sensor can't determine its location but does know when it overlaps a nearby sensor. We say that an evasion path exists in this sensor network if a moving evader can avoid detection. Using tools from topology, Vin de Silva and Robert Ghrist can guarantee that no evasion path exists in certain networks. But what about the remaining networks? We'll consider examples that show the existence of an evasion path depends not only on the sensor network's local connectivity data but also on its embedding.

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MS2

Generalizing Max Flow and Min Cut: Opportunities from a Topological Proof

The max-flow min-cut theorem has found recent applications in image segmentation, communication, and other forms of information processing. The classical theorem and its proof can be recast in terms of the "directed homology' of a directed graph, taking coefficients in a sheaf of constraints. I will discuss generalizations of max-flow min-cut implied by the topological approach, and potential applications of such generalizations to real-world problems.

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MS2

Sheaves and Persistence

Sheaf theory brings to persistence a rich language. Using this language, I will present, through simple examples, some ongoing work on multidimensional persistence.

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MS2

Recent Advances and Trends in Applied Algebraic Topology

Applied algebraic topology is a vibrant young field of research, with rapid ongoing development. I will give a survey of recent advances and results in the field including work on coordinatization, on topological inference, on topological simplification, and applications to signals, to cancer research, and to image analysis. I will focus, in this, on work done by young researchers in the field.

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MS3

Stable Computation with Reproducing Kernels

Positive definite kernels and their associated reproducing kernel Hilbert spaces provide a very flexible and powerful tool for the solution of many typical problems of numerical analysis and scientific computing such as function approximation, numerical integration or the numerical solution of PDEs. I will provide a brief introduction to positive definite reproduc- ing kernels, mention some typical applications, and then focus on stable computation with Gaussian kernels. The latter is motivated by the fact that, on the one hand, interpolation with flat Gaussian kernels provides a generalization of (multivariate) polynomial interpolation with spectral convergence rates for smooth functions, while, on the other hand, flat Gaussian kernels lead to notoriously ill-conditioned linear systems. Our work demonstrates that this so-called *uncertainty principle* can be avoided by representing the space of functions used for the approximation by a "better" basis. A set of MATLAB routines implementing these ideas for Gaussian kernels are available from http://math.iit.edu/˜mccomic/gaussqr

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MS3

Refinement and Remeshing in Particle Simulations

Lagrangian particle simulations are often used to study vortex dynamics in the context of incompressible fluids. It is well-known that the simulation accuracy is sensitive to the particle distribution, and maintaining a proper distribution as the flow evolves is a challenging problem. I'll discuss some techniques used to address this issue in two applications: (1) adaptive panel refinement for vortex sheets, and (2) particle remeshing for the barotropic vorticity equations on a rotating sphere.

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MS3

Multi-moment Vortex Methods

In this talk we develop a new, high order accurate, multi-moment vortex method (MMVM) using Hermite expansions to simulate 2D vorticity. The method naturally allows the particles to deform and become highly anisotropic as they evolve without the added cost of computing the non-local Biot-Savart integral. Convergence for the method is proven and examples will be provided. Time permitting, we will discuss the spatial accuracy and computational costs of MMVM.

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MS3

A Partition of Unity Method for Divergence-free Approximation of Vector Fields on the Sphere

Vector fields tangent to the surface of the sphere appear in many applications from the geophysical sciences. Often these fields describe the velocity of some incompressible fluid and are thus divergence-free. We present a new mesh-free, partition of unity method based on RBFs for approximating these types of fields that preserves the divergence-free property. The method is computationally efficient, free of any coordinate singularities, and can be used to approximate surface derivatives of the field.

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MS4

Development of a Single Domain Framework to Model 3D L-Ion Intercalation Batteries using the AMP Package

Modeling of batteries involves simulation of coupled charge and thermal transport, interfacial electrochemical reactions across the porous 3D structure of the electrodes (cathodes and anodes) and electrolyte system. The resulting equations are stiffff differential algebraic systems on a single domain and require a robust solution methodology. These formulations are implemented in AMPERES code, an external package for AMP software. In the talk we demonstrate the importance of the coupled solution procedure using Newton Krylov iterative solvers. Experiments based on various preconditioning strategies are presented.

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MS4

The Arctic Terrestrial Simulator: Developing a Flexible Multiphysics Simulator based on Amanzi

The Arctic Terrestrial Simulator (ATS) is being developed to simulate coupled processes governing carbon releases from degrading permafrost, including subsurface and overland flow, heat transport, subsidence, and soil biogeochemistry. A flexible simulation capability that naturally supports strong and weak coupling of selected processes is required. Building upon Amanzi, the ASCEM simulator, we present a general strategy for dynamically managing data structures, data permissions, and process model couplings for the ATS.

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MS4

A Multiphysics PDE Assembly Engine for Nonlinear Analysis using Template-based Generic Programming Techniques

As computational algorithms, hardware, and programming languages have advanced over time, computational modeling and simulation is being leveraged to understand, analyze, predict, and design increasingly complex physical, biological, and engineered systems. Because of this complexity, significant investments must be made, both in terms of manpower and programming environments, to develop simulation capabilities capable of accurately representing the system at hand. At the same time, modern analysis approaches such as stability analysis, sensitivity analysis, optimization, and uncertainty quantification require increasingly sophisticated capabilities of those complex simulation tools. Often simulation frameworks are not designed with these kinds of analysis requirements in mind, which limits the efficiency, robustness, and accuracy of the resulting analysis. In this work, we describe an approach for building a mulitphysics assembly engine that natively supports requirements for many types of analysis algorithms and solution techniques. This approach leverages compile-time polymorphism and generic programming through C++ templates to insulate physics experts from the complexities associated with the analysis hierarchy and solution techniques. The ideas presented here build on operator overloading-based automatic differentiation techniques to transform a simulation code into one that is capable of providing analytic derivatives. However we extend these ideas to compute quantities that aren't derivatives such as polynomial chaos expansions, floating point counts, and extended precision calculations. We will show example use cases including turbulent flow in a light water nuclear reactor, and stability analysis of a magnetohydrodynamics test problem.

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MS4

The Advanced Multi-Physics (AMP) Package With An Application to Fuel Assemblies in Nuclear Reactors

Simulations of multiphysics systems are becoming increasingly important in many science application areas. In this talk we describe the design and capabilities of the Advanced Multi-Physics (AMP) package designed with multidomain multi-physics applications in mind. AMP currently builds powerful and flexible deterministic multiphysics simulation algorithms from lightweight operator, solver, linear algebra, material database, discretization, and meshing interfaces. In this and related talks we will describe how AMP has been used to solve coupled multi-domain multiphysics problems related to energy applications.

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MS5

Advances on the Discretizable Distance Geometry Problem

The Discretizable Distance Geometry Problem (DDGP) is a subset of the DGP which can be solved using a discrete search occurring in continuous space. Its main application is to find three-dimensional arrangements of proteins using

NMR data. We will talk about our efforts that have been directed towards adapting the DDGP to be an ever closer model of the actual difficulties posed by the problem of determining protein structures from NMR data.

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MS5

Coarse Grained Normal Mode Analysis vs. Refined Gaussian Network Model for Protein Residue-Level Structural Fluctuations

We investigate several approaches to coarse grained normal mode analysis on protein residual-level structural fluctuations by choosing different ways of representing the residues and the forces among them. The residue mean-square-fluctuations and their correlations with the experimental B-factors are calculated for a large set of proteins. The extracted force constants from the Hessian are surveyed, and the statistical averages are used to build a refined Gaussian Network Model. Joint work with Robert Jernigan and Zhijun Wu.

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MS5

The Determination and Refinement of Protein Ensembles using Inter-atomic Distance Bounds

A novel approach is proposed for the determination of the ensemble of structures for a protein given a set of distance bounds from NMR experiments. In this approach, similar to X-ray crystallography, a protein is assumed to have an equilibrium structure with the atoms fluctuating around their equilibrium positions. Thus, the structure determination problem can be formulated as an optimization problem, i.e., to find the equilibrium positions and maximal possible fluctuation radii for the atoms in the protein, subject to the condition that the fluctuations should be within the given distance bounds. The advantages of using this approach are the following: (1) The mathematical problem to be solved becomes more tractable, and only a single solution to an optimization problem is required, while in conventional approaches, multiple solutions are sought for a system of inequalities, which in general is intractable. (2) A single structure along with the estimates on the atomic fluctuations suffices to describe the structure and its fluctuation ranges that are underestimated in conventional approaches using a finite number of structural samples. (3) A single structural model with the fluctuation radii corresponding to the B-factors can be obtained for the full description of an NMR structure and its dynamic properties, the same as in X-ray crystallography. The formulation of the optimization problem is given. The algorithm for solving the problem is described. The test results on model proteins are presented.

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MS5

An Optimal Solution to the Generalized Distance Geometry Problem

NMR experiments on a protein yield a set of inter-atomic distance ranges. A number of structures satisfying the distance constraints, derived from distance range and bond information, are then generated. This ensemble of structures is often under represented and inaccurately represents the protein's structural fluctuations. In this presentation we present an alternative problem where its solution, derived from interior point optimization, provides a single representation for a protein's conformation and its ensemble of possible structures.

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MS6

Homogenization-based Mortar Methods for Porous Media

For an elliptic problem with a heterogeneous coefficient in mixed form, nonoverlapping mortar domain decomposition is efficient in parallel if the mortar space is small. We define a new multiscale mortar space using homogenization theory. In the locally periodic case, we prove the method achieves optimal order error estimates in the discretization parameters and heterogeneity period. We assess its numerical performance when the coefficient is not locally periodic.

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MS6

Multiscale Model Reduction for Flows in Heterogeneous Porous Media

For multiscale problems, some types of coarsening of the detailed model are usually performed before the model can be used to simulate complex processes. In this talk, I will describe multiscale model reduction techniques that can be used to systematically reduce the degrees of freedoms of

fine-scale simulations and discuss applications to preconditioners. For parameter-dependent problems, I will describe how Reduced Basis approaches can be used offline to generate reduced local problems.

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MS6

An Exponentially Convergent Approximation Theory for Fields Inside Multiscale Heterogeneous Materials

Large multiscale engineering systems such as airplane wings and wind turbine blades are built from fiber reinforced composites and exhibit a cascade of substructure spread across several length scales from microns to tens of meters. The computational modeling of these hierarchical and heterogeneous structures is a very large problem that requires parallel computation. In this talk we address both the problems of parallelization and dimension reduction and present an exponentially convergent approximation theory for multiscale problems. This is joint work with Ivo Babuska and has appeared in Multiscale Modeling and Simulation, SIAM, (2011) 9, 373 406.

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MS6

Multiscale Mortar Coupling of Multiphase Flow and Reactive Transport on Non-matching Grids

Geochemical modeling plays an important role in designing carbon sequestration strategies, characterizing environmental site contaminations, and predicting environmental impacts. We formulate a multiscale model for coupling multiphase flow and reactive transport in porous media. The flow is modeled using mortar mixed finite elements that allow for accurate and efficient parallel domain decomposition with non-matching grids. The reactive transport equations are treated using operator splitting for decoupling transport and reactions. Computational results are presented.

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MS6

Modeling Flow and Coupled Transport with Adsorption from Pore to Core

Mathematical modeling of flow and transport in porous media until recently has been restricted to the scales of observation i.e. from core scale up. However various experimental techniques and discrete and continuum based computational methods are now available for the study of phenomena at porescale. Most interesting are coupled processes whose influence on the core and field scale flow and transport is essential but for which upscaled models, especially for high flow rates, are lacking. We discuss our recent results based on experimental as well as complex synthetic geometries.

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MS7

Composed Solution Methods for General Nonlinear Equations

The numerical solution of large-scale nonlinear systems of equations may be performed using Newton's method, global methods, like nonlinear Krylov methods, or local methods, like nonlinear Gauss-Seidel. Many problems cannot be efficiently solved using Newton-like schemes. As an alternative, we propose a flexible framework for the composition of local and global methods. We demonstrate the effectiveness and efficiency of composable nonlinear solvers on problems of interest from computational biology.

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MS7

Physics-based Preconditioning within Implicit Simulations of Visco-resistive Tokamak Plasmas

Single-fluid resistive magnetohydrodynamics (MHD) is a fluid description of fusion plasmas which is often used to investigate macroscopic instabilities in tokamaks. In MHD modeling of non-spherical tokamaks it is often desirable to compute MHD phenomena to resistive time scales, which can make explicit time stepping schemes computationally intractable. Our work focuses on simulations using a structured mesh mapped into a toroidal geometry with a shaped poloidal cross-section, and a finite volume spatial discretization of the PDE model. We discretize the temporal dimension using a fully implicit θ or BDF method, and solve the resulting nonlinear algebraic system using a standard inexact Newton-Krylov approach. The focus of this talk is on the construction and performance of physics-based preconditioning approaches for accelerating convergence of these iterative solvers. We compare preconditioners inspired by solvers from legacy MHD codes, though here they are used within a preconditioning context. We conclude with numerical results in the context of pellet-injection fueling of tokamak plasmas.

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MS7

Anderson Acceleration of Modified Picard Iteration for Variably Saturated Flow

We will present our investigation of the effectiveness of the Anderson Acceleration method applied to the modified Picard iteration for simulations of variably saturated flow. We solve nonlinear systems using both unaccelerated and accelerated modified Picard iteration as well as Newton's method. Since Picard iterations can be slow to converge, the advantage of acceleration is to provide faster convergence while maintaining advantages of the Picard method over the Newton method. Results indicate that the accelerated method provides a robust solver with significant potential computational advantages.

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MS7

An Optimal Convergence Neighborhood Strategy for an Implicit Timestep Solver That Converges All the Time

The Adaptively-Localized-Continuation-Newton (Younis, R.M. et al., 2008) method is a numerical continuation scheme that applies time-step size as its homotopy parameter. The solver unifies implicit time-stepping with nonlinear iteration. A key component that dictates a trade-off between efficiency and robustness is the choice of Convergence Neighborhood about the solution path. This work analyzes an automatically adaptive strategy for this choice in order to locally optimize the progress in time advancement while still guaranteeing unconditional robustness.

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MS8

A Multi-numeric Method for Convection-dominated Parabolic Problems Using an Adaptive Region-swapping Approach

This work couples the finite volume (FV) method with the discontinuous Galerkin (DG) method dynamically. For each time-step, an efficient partition of the domain between the two methods is determined in an attempt to best preserve the high accuracy of the DG method while also taking advantage of the low computational cost of the FV method wherever is possible. The implementation preserved the expected numerical convergence rates, while yielding substantially smaller linear systems. Advisor: Beatrice Riviere, Rice University

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MS8

Spectral Properties of Neural Network Structures

I investigate how biologically relevant patterns of network connectivity affect neural activity. To encode network structure, I construct synaptic weight matrices and observe changes in spectra and resulting dynamics. Differences in spectra for small world, nearest neighbor, and random networks affect prevalence of stable, periodic, and chaotic solutions, Lyapunov exponents, and frequencies measured by Fourier series approximations. The degree of asymmetry in the matrix affects radius, number of real eigenvalues, and types of chaos achieved. Advisor: Dr. Jonathan Rubin, University of Pittsburgh

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MS8

The Effects of Signal Delay in Gene Regulatory Networks

Delay can qualitatively affect the dynamics of gene regulatory networks. It has been shown that delay can cause oscillations and increase signal-to-noise ratios. Using analytical techniques, stochastic modeling, model reduction techniques, and simulations, we will study how delay affects the flow of information through gene regulatory networks. Advisor: William Ott, University of Houston

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MS9

Analysis of Nematic Liquid Crystals with Disclinations

We investigate the structure of nematic liquid crystal thin films described by the Landau-de Gennes tensor-valued order parameter for energy minimizers with Dirichlet boundary conditions of nonzero degree. We prove that as the elasticity constant goes to zero a limiting uniaxial texture forms with disclination lines corresponding to a finite number of defects, all of degree one-half or minus one-half.

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MS9
Ferronematic Liquid Crystal Composites

The coupling effects of nematic liquid crystals to magnetic fields are usually weak, due to the small values of the anisotropic diamagnetic susceptibility. In their seminal work, F.Brochard and P.G.de Gennes (Physique des Solides, 1970), investigated suspensions of magnetic grains in liquid crystals. We discuss the roles and interaction between theoretical and experimental research works in the ensuing decades, and present a mathematical justification of the proposed models.

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MS9
Recent Results on Nematic Elastomers

Abstract not available at time of publication.

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MS9
Electric-Field-Induced Instabilities in Liquid-Crystal Films

Simple models of liquid crystals characterize orientational properties in terms of a *director fie d*, which can be influenced by an applied electric field. The local electric field is influenced by the director field; so equilibria must be computed in a coupled way. Equilibria are stationary points of a *free energy functional*, which can fail to be coercive because of the nature of the director/electric-field coupling. We discuss characterizations of local stability and anomalous behavior in such systems.

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MS9
Extrinsic Curvature, and Two-dimensional Nematic Order

We derive two-dimensional free energies, aimed at describing the alignment of nematics deposited on curved substrates, from the conventional three-dimensional theories of nematic liquid crystals. Both the director and the order-tensor theories are taken into account. The so-obtained surface energies exhibit extra terms compared to earlier models. These terms couple the shell geometry with the nematic order parameters. As expected, the shape of the shell plays a prominent in the equilibrium configurations of nematics coating it.

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MS10
Characterization of Discontinuities in High-dimensional Stochastic Problems on Adaptive Sparse Grids

Stochastic collocation methods are an attractive choice to characterize uncertainty because of their non-intrusive nature. High dimensional stochastic spaces can be approximated well for smooth functions with sparse grids. There has been a focus in extending this approach to non-smooth functions using adaptive sparse grids. This presentation will present both adaptive approximation methods and error estimation techniques for high dimension functions.

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MS10
Sparse Grids for Uncertainty Quantification

This talk will discuss the use of sparse grids to approximate the high dimensional integrals that arise when uncertainty in problem inputs is modeled by assigning a probability density function over each range and considering the product space of all possibilities. We will consider generalizations of the sparse grid approach that place more emphasis on some input factors.

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MS10
An Efficient Sparse-grid-based Method for Bayesian Uncertainty Analysis

Abstract not available at time of publication.

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MS10
A Hierarchical Adaptive Sparse Grid Stochastic

Wavelet Collocation Method for PDEs with Random Input Data

Accurate predictive simulations of complex real world applications require numerical approximations to first, oppose the *curse of dimensionality* and second, converge quickly in the presence of steep gradients, sharp transitions, bifurcations or finite discontinuities in high-dimensional parameter spaces. In this talk we present a novel multidimensional multiresolution adaptive (MdMrA) sparse grid stochastic collocation method, that utilizes hierarchical multiscale piecewise Riesz basis functions constructed from interpolating wavelets. The basis for our non-intrusive method forms a stable multiscale splitting and thus, optimal adaptation is achieved. Error estimates and numerical examples will used to compare the efficiency of the method with several other techniques.

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MS11
Title Not Available at Time of Publication

Abstract not available at time of publication.

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Abstract not available at time of publication.

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MS11
Sheaves on Graphs

Abstract not available at time of publication.

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MS11
New Challenges in Cryptology

Abstract not available at time of publication.

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MS12
Panel Discussion: Teaming Up in Tough Times

This discussion section will be provide time for questions relating to the collaboration and opportunities that the speakers have addressed.

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MS12
Some Perspectives on Teaming from the DOE National Labs

I will present my perspectives on the role of teams in the current economic environment as we attempt to accomplish more science with scarcer resources and on what has been effective in forming and sustaining successful teams. I will call on my experiences in leading two multi-institutional mathematics teams for DOEs SciDAC program and my role as the division leader of a research organization charged with performing multidisciplinary research.

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MS12
Take Initiative, Make Contacts, and Collaborate: My Journey from Graduate Student to Professor

Being a successful mathematician involves more than just knowing the math. As in other professions, taking initiative and forming collaborations are crucial in a competitive job market. These strategies can be counter-instinctual and uncomfortable in male-dominant fields such as math. I will discuss my own strategies for overcoming unease in being aggressive. I will also share other strategies and mistakes that I made in transitioning from graduate student to professor.

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MS12
Building Relationships in the Tree of Life

The Tree of Life is a family tree showing the evolutionary relationships among all of the worlds organisms. I will discuss opportunities at the intersection of biology and computer science for constructing such an awesome representation of life. However, the Tree of Lifes impact transcends science. It may represent the ultimate role model for building connections in a sea of diversity.

Tiffani L. Williams

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MS13
Adaptive Magnetohydrodynamics Simulations with SAMRAI

A wide variety of plasma problems require both high resolution and large spatial domains that present a problem for existing models. Adaptive Mesh Refinement (AMR) provides an efficient method of obtaining both high resolution and a large spatial domain. AMR allows for both hi-resolution and large spatial domain computations. This talk will focus on using structured AMR with a 3D plasma model (pixie3d). Current progress will be presented.

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MS13
Composable Multilevel Methods for Multiphysics Simulations

Implicit solution methods for multiphysics problems are either monolithic (treating the coupled problem directly) or split (solving reduced systems independently), with multilevel methods often being important for algorithmic scalability in both approaches. We present flexible support developed in PETSc for block preconditioners, splitting in smoothers, related multiplicative relaxation, nonlinear and matrix-free variants, and communication/bandwidth reducing techniques. We demonstrate software modularity without sacrificing run-time algorithmic flexibility for applications in geodynamics and phase-field models.

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MS13
Tree Based Communication for Scalable Mesh Adaptation in the SAMRAI Framework

SAMRAI mesh adaptation involves collective, communication-intensive operations that are challenging to scale. The critical clustering and partitioning operations use virtual tree networks to limit communication latency to $\mathcal{O}(\log P)$ for P processes. However, ideal performance is hindered by a number of possible causes that are difficult to examine. In this work, we use newly developed tools to analyze the complex tree-based communications, with results leading to improved performance for SAMRAI applications.

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MS13
Building AMR into a Multiphysics Code Using the SAMRAI Framework

Supporting mature, evolving application requirements is a challenge for software frameworks. Using the SAMRAI framework, we have integrated adaptive mesh refinement (AMR) into a mature multiphysics code which is heavily used and under continual developed. SAMRAI provides unique object-oriented support for parallel AMR mesh and data management. We describe how SAMRAI allows decoupling AMR operations from the application mesh and data; SAMRAI does not own these entities, yet it manipulates them directly.

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MS14
Efficient Algorithms for Mesoscale Dynamics of Interacting Particle Systems

We present efficient algorithms for simulating evolution of space-time averages of large ODE systems. Averaging produces exact PDEs but they cannot be simulated without solving the underlying ODEs. We approximate these PDEs by new closed form equations that can be simulated independently of solving the underlying ODEs at a fraction of the cost. To achieve closure we use methods from the theory of ill-posed problems. We analyze quality of the approximation and efficiency of algorithms.

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MS14

Flux Norm and Finite-dimensional Homogenization Approximation with Non-separated Scales and High Contrast

In joint work with Owhadi we consider the most general case of arbitrary L^∞ coefficients, which may contain infinitely many scales not necessarily being well-separated. We establish a finite-dimensional homogenization approximation generalizing correctors in classical homogenization, and error estimates in the flux norm with an optimal error constant. We discuss recent results on localized multiscale basis and work in progress on compactness of the solution space, and new corrector results in classical periodic homogenization problem.

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MS14

Acoustic Propagation in a Saturated Piezo-Elastic, Porous Medium

We study the problem of derivation of an effective model of acoustic wave propagation in a two-phase, non-periodic medium modeling a fine mixture of linear piezo-elastic solid and a viscous Newtonian, ionic bearing fluid. Bone tissue is an important example of a composite material that can be modeled in this fashion. We develop two-scale homogenization methods for this system, and discuss also a stationary random, scale-separated microstructure.

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MS14

On the Integral Representation Formula (IRF) for a Two-parameter Family of Elastic Composites

This talk focuses on the derivation/implication of the IRF for two-phase composites in which the contrasts between two set of Lame coefficients can be described independently by the two parameters. This topic of research is inspired by the inverse problem of recovering microstructural information from measurement of effective properties of finely-structured composites (dehomogenization) in which IRF plays an essential role. This research is sponsored by ARRA-NSF-Math-Bio-0920852.

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MS15

Evolutionary Games with Gaussian Structures

We consider a population playing two-strategy symmetric games on a grid. A discrete Gaussian kernel rules out the interactions and information collection between individuals. We study how frequency and spatial structure of the population change over time for Prisoner's Dilemma game under four different update rules. Simulation results for these rules show frequencies of the games for kernels with different deviations. It is conjectured that, if the deviation of the kernel is large enough, bifurcation diagram of mean-field dynamics and spatial simulations agree. This result will be justified by showing the relation between macroscopic and mesoscopic limits of the same microscopic rule.

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MS15

Computation and Analysis of Evolutionary Game Dynamics

Biological species (viruses, bacteria, parasites, insects, plants, or animals) replicate, mutate, compete, adapt, and evolve. In evolutionary game theory, such a process is modeled as a so-called evolutionary game. We describe the Nash equilibrium problem for an evolutionary game and discuss its computational complexity. We discuss the necessary and sufficient conditions for the equilibrium states, and derive the methods for the computation of the optimal strategies, including a specialized Snow-Shapley algorithm, a specialized Lemke-Howson algorithm, and an algorithm based on the solution of a complementarity problem on a simplex. Computational results are presented. Theoretical difficulties and computational challenges are highlighted.

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MS15

Within-host Dynamics of Influenza Virus Infection with Immune Responses

Influenza virus infection remains a public health problem worldwide. The mechanism underlying viral control during an uncomplicated influenza virus infection is not fully understood. In this talk, I will address this question by developing mathematical models that include both innate and adaptive immune responses, and fitting them to experimental data. This study provides a quantitative understanding of the biological factors that can explain the viral and interferon kinetics during a typical influenza virus infection, and may provide more information for future research in influenza pathogenesis, treatment, and vaccination.

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MS15

Modeling the Dynamics of Cross-infection of Leishmania Amazonensis and Leishmania Major

Immune response during the course of *Leishmania* infection is a classical and crucial model in immunology and pathology, as it revealed and claried a large number of critical and essential immunology factors such as binary pathways of CD4+ T helper cells activations, transportation of pathogens by dendritic cells, and mechanisms of macrophage to clean the pathogens etc. Recently, a series of experiments on the cross infection of *Leishmania amazonensis* and *Leishmania major* on C3HeB/FeJ and C57BL/6 mice [Jones et.al. 06, 11] indicates critical functions of B cells during the process of cleaning the pathogen and resolving the no-healing diseases caused by *Leishmania amazonensis*. Those experimental results also demonstrate interesting population dynamics that the two strains of *Leishmania* interact indirectly through inducing different immune responses. Using immunobiological dynamics approach and game-theoretical approach, we propose and compare two mutually different models to study the cross infection of *Leishmania amazonensis* and *Leishmania major* based on [Jones et.al. 06, 11]. Detailed analysis and numerical simulation are conducted based on parameters identified from the data.

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MS16

Root Counts, Eigenvectors and Numerical Homotopies

We will explain how solutions to polynomial systems can be viewed as zero sets of sections of vector bundles with the result of reducing the number of homotopy paths used in a numerical solution of the system. Specifically we will look at the tangent bundle of projective space and associated systems of polynomials. We anticipate that solving these polynomial systems numerically amounts to a numerical method to compute the Jordan canonical form of a matrix.

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Chris Peterson
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MS16

Filtering Homotopies for Discretized Boundary Value Problems

Discretizations of boundary value problems arising from models in science and engineering often yield polynomial systems. Homotopy continuation methods allow one to compute all solutions on a given mesh, but even a moderate size grid may lead to an intractably high degree system. However, generally most of the solutions are nonphysical, and so filtering techniques aim to reduce the work spent on them. In this talk we discuss a new approach for forming filtering homotopies over a continuous family of numerical schemes, which in turn allows for more robust filtering criteria and less reliance on ad hoc threshholds.

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MS16

Real Algebraic Geometry in Combinatorics

The talk will give an overview of several problems in Geometric Combinatorics and will describe some approaches to these problems through Real Algebraic Geometry.

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MS16

Building a User Friendly Matlab Platform for Numerical Polynomial Algebra

Numerical polynomial algebra and numerical algebraic geometry has enjoyed tremendous advancement in recent years with many algorithms becoming standard. A Matlab package Apalab, initially developed several years ago for numerical polynomial algebra, is in major upgrade. In additional to adding algorithms/implementations, we are designing an intuitive interface so that casual users and early students can engage advanced polynomial computation easily. This talk will present those new developments toward building such a Matlab platform.

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MS17

Improvements in Adaptive Nonlinear Filtering in Regularization Models for Incompressilbe Flows

We will review some recent results for adaptive nonlinear filtering in regularization models of incompressible flow. We will then discuss some improvements in how to define the indicator functions. We will present a numerical method using these ideas, prove convergence of it to the model, and give several test examples.

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MS17

A Least Squares Approach for the Coupled Stokes-

Darcy System

We consider a linear/nonlinear Stokes flow coupled with a porous medium flow with only flow rates specified on the inflow and outflow boundaries in both flow domains. The coupled Stokes-Darcy system is formulated as an optimal control problem where a common force is used as a control to minimize the the jump in normal velocities of two flows across the interface and to match the given flow rates. We analyze the optimal control problem and use a least squares approach for which a Gauss-Newton type algorithm is considered. Numerical results are presented to validate convergence of the algorithm.

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MS17
Coupling Biot and Navier-Stokes Equations for Modelling Fluid-poroelastic Media Interaction

The interaction between a free fluid and a deformable porous medium is found in a wide range of applications: ground-surface water flow, geomechanics or blood-vessel interactions. We focus on the latest application. The fluid-poroelastic structure interaction (FPSI) problem in hemodynamics couples the Navier-Stokes equations for an incompressible fluid to the Biot problem, the latter governing the motion of a saturated poroelastic medium. Only a limited number of works deal with this problem. The finite element approximation of the FPSI problem is involved due to the fact that both subproblems are indefinite. We introduce a residual-based stabilization technique for the Biot system, motivated by the variational multiscale approach. This technique allows the use of the same finite element spaces for all the velocities and pressures, greatly simplifying the discretization and the enforcement of coupling conditions. We choose a fixed point method for the linearization of the Navier-Stokes/Biot coupled system. To solve the linear FPSI system at every fixed point iteration, we propose to use both a monolithic approach and partitioned procedures based on domain decomposition preconditioners (the Dirichlet-Neumann, Robin-Robin, and Robin-Neuman ones). We compare the efficiency of all the methods on a test problem. The performance of the monolithic approach improves as the added-mass effect gets critical and the Robin-Neumann preconditioner proves to be the less sensitive to the added-mass effect.

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MS17
Multiscale Deconvolution Models of Turbulence

We will prove several mathematical and physical properties for the newly developed (A. Dunca, 2011) multiscale-deconvolution models of turbulence. We prove conservation laws, derive a microscale, and show the existence of global attractors. Additionally, we derive a numerical scheme for the model, and show results of preliminary tests on some benchmark problems.

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MS18
Mathematical Models of Gels in Biomedical Applications: Drug Delivery Devices

Abstract not available at time of publication.

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MS18
Immersive Visualization and Computational Creativity for Biomedicine

This talk will focus on recent advances in interactive visualization in immersive virtual reality and on the emerging research topic of computational creativity the development of computer tools for supporting creative human tasks, such as 3D design. Exciting recent interdisciplinary applications of this research to biomedicine at the University of Minnesota will be described, including research on a new multi-touch 3D visualization environment for designing medical devices within virtual models of the human anatomy.

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MS18
Tracking Brain and CSF Evolution via Level Set/mesh Warping Algorithm during Hydrocephalus Treatment

Hydrocephalus is a serious neurological disorder in which there is an abnormal accumulation of cerebrospinal fluid (CSF) in the brain ventricles, causing brain enlargement and tissue compression. Although hydrocephalus treatment has been performed by surgical CSF shunt insertion, computational models are needed to track hydrocephalic brain movement. Thus, we propose a combined level set/mesh warping algorithm and use it to simulate the evolution of the brain ventricles and the CSF in pedi-

atric hydrocephalic patients.

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MS18

Immunotherapy and Aging Effects in Immune Modulated Tumor Growth

The presence of cancer in a host elicits an immune response that can be both inhibitory and stimulatory to tumor development. Aging decreases the effectiveness of the immune response, which can alter immune modulation of tumor growth. We present a mathematical model based on principles of generalized logistic growth that incorporates both pro- and anti-tumor immune processes. We then use this model to investigate the effects of aging and immunotherapy on tumor development.

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MS19

Symplectic Methods for an Exactly Solvable Kolmogorov Model of Two Interacting Species

We discuss the behavior of symplectic integration methods for an exactly solvable Kolmogorov predator-prey model of two interacting species. Using numerical experiments, we investigate the accuracy, conservation, and periodic orbits of this Hamiltonian system. In light of this, we present potential generalizations to other population dynamics with bounded state variables. Advisor: Ari Stern, University of California, San Diego

Katherine Ball
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MS19

CGPOP Analysis and Optimization

The CGPOP miniapp is the conjugate gradient solver from Los Alamos National Laboratory's Parallel Ocean Program (POP) version 2.0. It includes several algorithms with combination of different communication modes and task partition strategies. The main goal of the project is to study and to improve the performance the methods. It involved the installation, execution, performance measurement and evaluation, modification and improvement to the code of CGPOP. Students obtained better understanding on parallel computing after working on the project. Advisors: Xiaoge Wang, Yinsheng Ji, Cheng Zhang

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MS19

Periodic Dispersion

The evolution of linearly dispersive equations with piecewise constant initial data on periodic domains depends on the asymptotic behavior of the dispersion relation. In particular, dispersion relations with asymptotically polynomial growth lead to dispersive quantization, being (approximately) quantized at rational times but fractal at irrational times. Similar phenomena are known as Talbot effect in optics and quantum mechanics. Numerical experiments and some analysis indicate that such effects persist into the nonlinear regime. Advisor: Peter J. Olver, U Minnesota

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MS19

Modeling Earth's Temperature and Atmospheric Carbon Dioxide

From ice core data, it is known that over the past 400,000 years, surface temperatures and atmospheric CO2 concentrations have oscillated with a period of approximately 100,000 years. The model introduced by Budyko (1969) is a simple model for the temperature of the Earths surface, but it does not allow atmospheric CO2 to change. Here, the Budyko model is altered to allow CO2 to change, so as to explore the interactions between CO2 and temperature. Advisor: Mary Lou Zeeman

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MS20

Multiscale Models for Coupled Flow and Elasticity

In this talk, a multiscale framework for fluid-structure interaction problem in an inelastic media is developed and analyzed. We assume Stokes flow at the pore scale and an elasticity model for pore-level deformations. Because of the complexity of the interaction at the pore level, an iterative macroscopic model is proposed. The constitutive relations representing media deformation is modeled via an iterative procedure. Constitutive equations are derived. Numerical results are presented.

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MS20

Advanced Discretizations for Modeling Flow and Reactive Transport on Highly Distorted Unstructured Grids

Abstract not available at time of publication.

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MS20

Coupled and Hybrid Models for Methane Evolution in Subsurface

We discuss challenges in computational modeling of processes of multicomponent adsorption and phase change coupled to flow and transport processes in coalbed methane and undersea methane hydrates. We report on our recent results on i) implementation of solvers for PDEs with constraints which are necessary for continuum level models, ii) handling multiscale processes in micropores using discrete scale models, and iii) modeling of pore- to core- couplings in hybrid models which bridge between continuum and discrete scales.

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MS20

Analysis of CO2-water Models

Abstract not available at time of publication.

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MS20

Coupling Compositional Flow, Transport, and Mechanics in Porous Media for Modeling Carbon Sequestration in Saline Aquifers

A key goal of our work is to produce a prototypical computational system to accurately predict the fate of injected CO2 in conditions governed by multiphase flow, rock mechanics, multi-component transport, thermodynamic phase behavior, chemical reactions within both the fluid and the rock, and the coupling of all these phenomena over multiple time and spatial scales. Even small leakage rates over long periods of time can unravel the positive effects of sequestration. This effort requires high accuracy in the physical models and their corresponding numerical approximations. For example, an error of one percent per year in a simulation may be of little concern when dealing with CO2 oil recovery flooding, but such an inaccuracy for sequestration will lead to significantly misleading results that could fail to produce any long-term predictive capability. It is important to note that very few parallel commercial and/or research software tools exist for simulating complex processes such as coupled multiphase flow with chemical transport and geomechanics. Here we discuss modeling multicomponent, multiscale, multiphase flow and transport through porous media and through wells and that incorporate uncertainty and history matching and include robust solvers. The coupled algorithms must be able to treat different physical processes occurring simultaneously in different parts of the domain, and for computational accuracy and efficiency, should also accomodate multiple numerical schemes. We present results demonstrating accuracy of schemes as well as applications from the Cranfield Mississippi demonstration site and core scale experiments.

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MS21

Bending, Twisting, and Snapping: Mechanics and Dynamics of Slender Structures

Soft materials undergo volume changes and instabilities when subjected to external stimuli. These instabilities and bifurcations can lead to dynamical shape changes in the morphogenesis in growing soft tissues. In this work, we present the dynamic instabilities that occur by straining an elastomer nonhomogenously with a favorable solvent. We examine how thin elastic plates undergo rapid bending, twisting, and snap-buckling instabilities when swollen.

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MS21

An Electromechanical Model of Tubular Heart Pumping in Ascidians

Recent advancements in computational fluid dynamics have enabled researchers to efficiently explore problems such as insect flight and fish swimming that involve moving elastic boundaries immersed in fluids. These advances have also made modeling the interaction between a fluid and an elastic model of an organ that includes some aspects of its physiology feasible. This presentation focuses on the development and implementation of coupled immersed boundary and electromechanical models of the tubular hearts of Ascidians.

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MS21

Anisotropic Diffusion in Swelling Polymer Gels

When anisotropic diffusion is taken into account, special forms of the diffusivity tensor $\mathbf{D}$ have to be taken into account, with $\mathbf{D} = \hat{\mathbf{D}}(\mathbf{d})$ and $\mathbf{d}$ the unit vector identifying the preferential (higher diffusivity) direction of diffu-

sion. The solvent flux $\mathbf{h} = -\mathbf{D}\nabla\mu$ which drives the solvent balance equation, coupled with the equations of the nonlinear three-dimensional elasticity, induces mechanical anisotropy, as evidenced in (DiMeo et al., Soft Matter 7, 6068, 2011). In this work, a few numerical simulations are carried out to investigate some significant cases.

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MS21
Nanoscale Mechanics of Natural Soft Materials

Nature requires soft tissue, e.g., elastomeric proteins or lipid layers, to be mechanically stable as they perform different tasks. In many cases, it has not been possible to replicate their mechanical properties in synthetic materials due to a lack of fundamental understanding of the mechanisms that the natural materials use. We present a novel insight into the behavior of natural soft materials through molecular mechanics simulations.

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MS22
Parametric and Other Exact Solutions to Einsteins Equations in Terms of Special Functions

In certain cosmological models the Einstein equations of general rel- ativity reduce to a differential equation whose solutions can be found in terms of Jacobi or Weierstrass elliptic functions. In recent joint work with Floyd L. Williams we find more widespread applications of spe- cial functions for other cosmological models. I will give an overview of techniques we employed in finding such special solutions that may be of use to a more general audience.

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MS22
A Method for Earthquake Cycle Simulations

We are developing a method to understand and simulate full earthquake cycles with multiple events on geometrically complex faults, with rate-and-state friction and off-fault plasticity. The method advances the model over long interseismic periods using the quasi- static equations, and through dynamic rupture using the elastodynamic formulation. To obtain an efficient and provably strictly stable method, we use high-order summation-by- parts finite difference schemes and weak enforcement of boundary conditions through the simultaneous approximation term.

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MS22
A Gamma-Convergence Analysis of the Quasicontinuum Method

Continuum mechanics models of solids have certain limitations as the length scale of interest approaches the atomistic scale. A possible solution in such situations is to use a pure atomistic model. However, this approach could be computational prohibited as we are dealing with billion of atoms. The quasicontinuum method is a computational technique that reduces the atomic degrees of freedom. In this talk, we review the quasicontinuum method and present a Gamma-convergence analysis of it.

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MS22
Video Stabilization of Atmospheric Turbulence Distortion

The image or the video sequence captured in a long-range system, such as surveillance and astronomy, is often corrupted by the atmospheric turbulence degradation. We propose to stabilize the video sequence using Sobolev gradient sharpening with the temporal smoothing. One latent image is found further utilizing the lucky-region method. With these methods, without any prior knowledge, the video sequence is stabilized while keeping sharp details and the latent image shows more consistent straight edges.

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MS23
Hom-Polytopes

Given full-dimensional polytopes P in R^p and Q in R^q, the *hom-polytope* $\mathrm{Hom}(P, Q)$ is defined to be the set of affine maps $L : R^p \to R^q$ such that $L(P)$ is contained in Q. It is not difficult to specify the facets of Hom(P,Q), but little else is known. We prove some categorical properties and produce a range of examples in low dimensions. Even when P and Q are polygons, the number of vertices of the hom-polytope depends on the geometry of P and Q, not just on m and n. We provide experimental results for pairs of regular polygons and a structural result for generic pairs of polygons.

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MS23

The Combinatorial Commutative Algebra of Conformal Blocks

Vector spaces of conformal blocks are objects from conformal field theory which have made surprising appearances in several moduli problems from algebraic geometry. We discuss the combinatorics underlying the dimension formulas of these spaces, and answer some questions about a classical moduli space: the moduli of rank 2 parabolic vector bundles on a projective algebra curve. In particular, we will use a polyhedral description of conformal blocks to construct presentations for coordinate rings of these spaces.

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MS23

Geometry of Exceptional Divisors and the Goemans-Williamson Algorithm

By a result of Mukai we can associate to each Dynkin diagram $T_{a,b,c}$ an algebraic variety $X_{a,b,c}$ whose geometry is controlled by the combinatorics of its (finitely many) exceptional divisors. In this talk we ask the question of determining the maximum number of pairwise intersections between two disjoint sets of such divisors. We give lower and upper bounds for this quantity and show that our bounds are asymptotically exact for the infinite families. Our results are a consequence of a detailed analysis of the behavior of the Goemans-Williamson random semidefinite approximation algorithm for the maxcut problem on strongly regular multigraphs.

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MS23

Singularities of Schubert and Richardson Varieties

This talk addresses the problem of how to analyze and discuss singularities of a variety X that "naturally' sits inside a flag manifold. Our three main examples are Schubert varieties, Richardson varieties and Peterson varieties. The overarching theme is to use combinatorics and commutative algebra to study the *patch ideals*, which encode local coordinates and equations of X. Thereby, we obtain formulas and conjectures about X's invariants. We will report on projects with (subsets of) Erik Insko (U. Iowa), Allen Knutson (Cornell), Li Li (Oakland University) and Alexander Woo (U. Idaho).

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MS24

A Multiscale Method Coupling Network and Continuum Models in Porous Media

In this talk, we present a numerical multiscale method for coupling a conservation law for mass at the continuum scale with a discrete network model that describes the pore scale flow in a porous medium. We developed single-phase flow algorithm and extended it to two-phase flow, for the situations in which the saturation profile go through a sharp transition from fully saturated to almost unsaturated states. Our coupling method for the pressure equation uses local simulations on small sampled network domains at the pore scale to evaluate the continuum equation and thus solve for the pressure in the domain. We present numerical results for single-phase flows with nonlinear flux-pressure dependence, as well as two-phase flow.

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MS24

Effective Properties of a Periodic Lattice of Circular Inclusions

The problem of determination of effective properties (conductivity, permittivity, etc.) of a medium containing an arbitrary doubly periodic array of identical circular cylinders within a homogeneous matrix is considered. We construct a quasiperiodic potential and determine the average field in the medium. The problem is then reduced to solution of an infinite system of linear equations. The effective conductivity tensor is obtained in the form of the series expansion in terms of the volume fraction of the cylinders whose coefficients are determined exactly. Results are illustrated by examples.

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MS24

Correctors and Field Fluctuation for the p(x)-Laplacian with Rough Exponents with Sub-Linear Growth

A corrector theory for the strong approximation of fields inside composites made from two materials with different power law behavior is provided. The correctors are used to develop bounds on the local singularity strength for gradient fields inside microstructured media. The bounds are multiscale in nature and can be used to measure the amplification of applied macroscopic fields by the microstructure. The talk will focus on the case of exponents with sublinear growth.

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MS24

Inverse Born Series for the Calderon Problem

We propose a direct reconstruction method for the Calderon problem based on inversion of the Born series. We characterize the convergence, stability and approximation error of the method and illustrate its use in numerical reconstructions.

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MS25

Efficient Computational Methods for Thermal Imaging of Small Cracks in Plates

We present some fast computational methods and practical considerations for identifying cracks in a two-dimensional plate using thermal data from an infrared camera, based on the "small volume expansions' developed Ammari, Vogelius, et. al. For an applied heat flux, the plate temperature is measured over its entire surface, so we have interior data, not just on the boundary. The novelty is that the cracks we seek are near or below the single-pixel resolution of the camera.

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MS25

Stochastic and Deterministic Inverse Solutions for Crack and Corrosion Imaging

Interesting mathematical issues arise when imaging tiny cracks and hidden corrosion in engineering applications using thermography. Sparse and noise pixel data "conspire' with the inverse heat (parabolic) operator to furnish an array of practical imaging challenges. This talk will explore deterministic and stochastic approaches to ameliorate such difficulties and discuss the algebraic and topological considerations that effect posedness in the deterministic case, and informativeness within the stochastic context.

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MS25

Application of Sparse Solutions to Underdetermined Problems in Imaging

The principle of parsimony has recently been demonstrated useful in solving highly underdetermined systems of linear equations. We first review the mathematics that make such solutions possible and then provide several applications of sparse (parsimonious) models in imaging. In the first we present results from the field of compressive sampling and show how high-fidelity imagery can be recovered from low-fidelity measurements. We then demonstrate how to develop and use sparse image models for image processing.

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MS26

Statistical Models and Methods for Anomaly Detection in Large Graphs

Traditional statistical models and methods provide a powerful framework for analyzing observed data. To extend these approaches to large graph-valued data sets, however, we must address significant theoretical and computational challenges. In this talk, we discuss new techniques for statistical inference on large graphs, with application to the detection of anomalous behavior in a citation database.

Nicholas Arcolano
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MS26

Streaming Graph Analytics for Massive Graphs

Emerging real-world graph problems include detecting community structure in large social networks, improving the resilience of the electric power grid, and detecting and preventing disease in human populations. The volume and richness of data combined with its rate of change renders monitoring properties at scale by static recomputation infeasible. We approach these problems with massive, fine-grained parallelism across different shared memory architectures both to compute solutions and to explore the sensitivity of these solutions to natural bias and omissions within the data.

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MS26

Perfect Power Law Graphs: Generation, Sampling, Construction and Fitting

Power law graphs are ubiquitous and arise in the Internet, the Web, citation graphs, and online social networks. Deviations from the power law model do not have a large impact on the qualitative characterization of graphs. However, the need for precise background models becomes essential in order to apply rigorous statistical signal processing techniques to detect graph anomalies. This work explores the power law degree distribution that is used to model power law graphs. A simple heuristic for generating perfect power law graphs is presented that reproduces many observed phenomena. Using this model the sampling effects of graph construction and edge ordering are examined. Graph construction appears to be a lossy, non-linear process that generates many phenomena that are observed in real data (e.g., data bin scatter, low-degree tails, and high-degree tails). Likewise, the order that edges are generated can have a strong effect on the evolution of the power law slope and the overall density of the graph (i.e., densification). Applying the perfect power law model to real data (e.g., entities extracted from the Reuters Corpus) provides a self-consistent set of degree bins for measuring deviations from the background. Using this scheme it is possible to identify specific edges that are typical, surplus, or deficit using standard signal processing techniques.

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MS26

Fast Counting of Patterns in Graphs

The occurrence of small subgraphs is a key ingredient in understanding real networks, since local interactions can reveal a lot of information about the full graph. For instance, the number of triangles indicates how well the graph is clustered. However, counting such small graphs can be computationally intensive, preventing adoption of such techniques on massive graphs. We are developing sampling-based algorithms for counting small sugbgraphs graphs. In this talk, we will present our latest results.

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MS27

High Order Mimetic Methods on a Nonuniform Mesh

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

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MS27

Mimetic Library Toolkit

Mimetic Methods Toolkit (MTK) is an application programming interface that allows the intuitive implementation of Mimetic Discretization Methods for the solution of Partial Differential Equations. Mimetic Methods yield numerical solution that guarantee uniform order of accuracy all along the modeled physical domain, while ensuring the satisfaction of conservative laws. Therefore, the attained numerical solutions remain physically faithful to the underlying physics of the problem. MTK is fully developed in ISO C++, thus exploiting all the well-known advantages of Object Oriented Applications as for example, providing the developer an intuitive perspective of the theoretical framework of Mimetic Discretization Methods. Likewise, Object Orientation carries along the advantages of the extensive collection of data structures manipulation capabilities of C++, thus allowing for a clearer programming methodology making MTK suitable for developing high-end scientific applications

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MS27

A Discrete Vector Calculus in Tensor Grids

The key to the success of mimetic discretization methods is that they discretize some description of continuum mechanics, e.g. vector calculus or differential forms. For a discretization to be fully mimetic it must have exact discrete analogs of the important results from the continuum theory. We summarize exactly which results from vector calculus are needed to derive energy inequalities for common initial boundary value problems, which we call the mimetic properties, and then produce a discrete vector calculus on tensor product grids in three dimensions that is fully mimetic.

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MS27

The Mimetic Spectral Element Method in the Community Atmosphere Model (CAM)

We describe a mimetic formulation of the spectral element method and its implementation in the the Community Atmosphere Model (CAM). For the atmospheric hydrostatic primitive equations, the mimetic properties of the method allow for excellent conservation on the unstructured, curvilinear meshes used by CAM. This includes local conservation (to machine precision) of quantities solved in conservation form, and semi-discrete conservation (exact with exact time-discretization) of derived quantities such as energy and potential vorticity.

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MS28

Defective Boundary Conditions for Viscoelastic Flow Problems

Abstract not available at time of publication.

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MS28

An ANOVA-based Method for High-dimensional

Stochastic PDEs

The Analysis of Variance (ANOVA) expansion is often used to reduce the cost of evaluating multivariate functions in high dimensions. We propose an ANOVA-based method for representation of multivariate functions, which does not depend on the choice of the anchor point, and tracks all the important parameters and important interactions, constructing the expansion with the minimum of the needed terms. We demonstrate a real life application where our method is the only usable approach.

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MS28

Analysis of Long Time Stability and Errors of Two Partitioned Methods for Uncoupling Evolutionary Groundwater - Surface Water Flows

Abstract not available at time of publication.

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MS28

An Adaptive Approach to PDE-constrained Optimization for Random Data Identification Problems

In this talk we will present a scalable mechanism for optimal identification of statistical moments or even the whole probability distribution of input random data, given the probability distribution of some response of a system of PDEs. This novel technique integrates an adjoint-based deterministic algorithm with the sparse grid stochastic collocation FEM. Our rigorously derived error estimates and several numerical examples, will be described and used to compare the efficiency of the method with several other techniques.

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MS29

Data Assimilation in Cardiovascular Mathematics: Toward An Integration of Patient-Specific Measurements and Simulations

In cardiovascular sciences, images and measures provide patient-specific knowledge that can enhance significantly the reliability of numerical simulations by proper data assimilation procedures. We address here the variational assimilation of velocity data and images for the accurate estimation of hemodynamics indexes of interest with both a deterministic and a Bayesian approach. The latter provides a better quantification of uncertainty and confidence regions for the quantities of interest.

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MS29

Fast Algorithms for Biophysics-based Medical Image Analysis

Abstract not available at time of publication.

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MS29

Patient-specific Mesh Generation for Improved Pulmonary Embolism Prevention

Pulmonary embolism is a potentially fatal disease involving the blockage of an artery of the lungs, typically by a blood clot. One treatment is via implantation of a mechanical device known as an inferior vena cava filter which traps large blood clots, preventing them from reaching the lungs. In this talk, we present a computational pipeline for generation of patient-specific meshes for use in CFD studies of blood flow for improved prevention of pulmonary embolism.

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MS29

Resolving Topology Ambiguity for Complicated Domain

We discuss all possible topology configurations and develop

an extension of the dual contouring (DC) method which guarantees the correct topology. We analyze all the octree leaf cells, and categorize them into 31 topology groups by computing the values of their face and body saddle points based on a tri-linear representation. Knowing the correct categorization, we are able to modify the base mesh and introduce more minimizer points to preserve the correct topology.

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MS30

Results from the Early Science High Speed Combustion and Detonation Project

The High Speed Combustion and Detonation project uses an adaptive mesh refinement, reactive flow Navier-Stokes code augmented with the equation of state, microscopic transport, and chemical kinetics required to study the detonation-to-deflagration transition in hydrogen. To run on future hardware, we have implemented mixed MPI/OpenMP threading, and parellelized the adaptive mesh refinement code. Our challenge is maintaining computational work load balance, and managing the distribution of ghost cells for communications performance.

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MS30

Implementing Hybrid Parallelism in FLASH

FLASH is a component-based multiphysics scientific software which has been used for computations on some of the largest HPC platforms. Simulation of turbulent nuclear combustion, a key process in Type Ia supernovae, is one of the target applications on the BG/Q platform at ANL. In preparation, we have introduced hybrid parallelism to the code. We describe these modifications, and also characterize the performance of the modified code on our first BG/Q racks.

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MS30

A Trillion Particles: Studying Large-Scale Structure Formation on the BG/Q

The simulation of structure formation in the Universe sits at the forefront of large-scale high-performance computing. I will discuss the unique algorithmic features employed on the BG/Q in HACC, our simulation code framework for computational cosmology, focusing on the way in which the gravitational force is divided into short range and long range components and how each component is efficiently and scalably computed using both inter- and intra-node parallelism.

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MS30

Automatic Generation of the HPCC Global FFT for BlueGene/Q

We present the automatic synthesis of the HPC Challenge's Global FFT, a large 1D FFT across a whole supercomputer system. The code was synthesized with the autotuning system Spiral. We run our optimized Global FFT benchmark on up to 128k cores (32 racks) of ANL's BlueGene/P "Intrepid' and achieved 6.4 Tflop/s. Further, we discuss the necessary changes for BlueGene/Q. Our BG/P code was part of IBM's winning 2010 HPC Challenge Class II submission.

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MS31

Shape Optimization of Plasmonic Gratings

Surface plasmons are electromagnetic fields, highly localized near metal- dielectric interfaces, and associated with surface electron density oscillations. We consider a problem of shape design of a metallic grating interface, so that surface plasmon modes are optimized. Existence and stability of optimal solutions is analyzed, and a gradient-based approximate solution method proposed. A numerical implementation which is capable of continuously tracking a changing grating interface is described, and numerical examples are presented.

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MS31

Overview of Shape Optimization Problems Involving Eigenvalues

Shape optimization problems involving eigenvalues arise in many areas where one seeks to control wave phenomena, including mechanical vibration in structures, electromagnetic waves in cavities, and population dynamics. We'll begin this minisymposium with an overview of the field and survey recent results on shape and structural eigenvalue optimization problems. In particular, well discuss Krein's now classic problem on the optimal density distribution of a membrane which extremizes the k-th Dirichlet-Laplacian eigenvalue.

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MS31

Asymptotic Calculation of Resonances

This work is motivated by the desire to develop a method that allows for easy and accurate calculation of complex resonances of a one-dimensional structures. We illustrate our approach for Schrodinger's equation whose potential is a low-energy well surrounded by a thick barrier. The resonance is calculated as a perturbation of the associated bound state when the barrier thickness is in fnite. We show that the error of this perturbational approach is exponentially small in barrier thickness. A similar result has been obtained for the case of a one-dimensional finite photonic bandgap structure with a defect. This is joint work with D. Dobson, J. Lin, S. Shipman, and M. Weinstein.

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MS31

Topology Optimization for Wave-Propagation Problems

The topology optimization method, originally developed for static mechanical problems, has in recent years been applied to a number of different inverse problems involving wave-propagation. The problem formulation makes use of element-based design variables and includes robustness towards manufacturing variations. The presentation will review the TopOpt-groups (www.topotp.dtu.dk) recent works within systematic design of: slow light photonic crystal waveguides; optic and acoustic cloaking devices; as well as structured surfaces for manipulation of visual appearance.

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MS32

Mathematical Modeling of Panama Disease in Cavendish Bananas Plants

The Cavendish banana has served global consumers for half a century and has remained unaffected by most types of Panama diseases. Currently, one type of Panama disease, fusarium oxysproum f.sp. cubense, targets the Cavendish banana. We propose a simple mathematical system of ordinary differential equations, based on an SI epidemic model, describing the interactions between susceptible and infected bananas. To lengthen survival of healthy bananas plants, infected bananas plants are removed from plantations. In our study, we consider various harvesting parameter values and present preliminary numerical results.

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MS32

Simulation of Deformations and Shape Recovery of Red Blood Cells Using the Lattice Boltzman Method

Red blood cells (RBCs) undergo substantial changes of shape during blood flow in vivo. In the past decade, Lattice Boltzmann and Immersed Boundary methods have been used to simulate the deformation of RBCs (e.g., Sui et al, IJMPC, 2007). We introduce a more comprehensive version of these models, aimed at simulating the shape recovery of a deformed RBC. Benchmarks and preliminary results of the model are introduced.

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MS32

Modeling of the Dynamic Delamination of L-

shaped Unidirectional Laminated Composites

One of the widely used geometrically complex parts in advanced commercial aircraft is the L-shaped composite. Due to the sharp curved geometry, interlaminar opening stresses are induced and delamination occurs under considerable mode-mixities in L-shaped beams. Dynamic phenomena during delamination initiation and propagation of L-shaped beams are investigated using dynamic (explicit) finite element analysis in conjunction with cohesive zone methods. The 2-D model consists of 24 plies of unidirectional CFRP laminate with an initial 1 mmcrack at the center of the laminate at the bend. Loading is applied parallel to one of the arms quasi-statically. The loading type yields different traction fields and mode-mixities in the two sides of the crack in which delamination occurs under shear stress dominated loading on one crack tip and opening stress dominated loading on the other. The speed of the delamination under shear dominated loading at one side is 800 m/s and under normal stress dominated loading is 50 m/s. In addition radial compressive waves at the interface are observed. Finally, as the thickness is changed, a different failure mode is observed in which a secondary crack nucleates at the arm and propagates towards the center crack.

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MS32

Numerically Optimal High Order Strong Stability Preserving Multi-step Runge-Kutta Methods

We investigate the strong stability preserving (SSP) property of multi-step Runge–Kutta (MSRK) methods with 2-6 steps. Whereas explicit SSP RungeKutta methods have order at most four, explicit SSP MSRK methods break this order barrier. We present our algorithm for finding numerically optimal explicit MSRK methods, and methods of up to five steps and eighth order that were found using this algorithm. These methods have larger SSP coefficients than any known methods of the same order of accuracy, and may be implemented in a form with relatively modest storage requirements. The usefulness of the MSRK methods is demonstrated through numerical examples, including integration of very high order WENO discretizations.

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MS32

Simulating Two-Phase Flows in Fractured Reservoirs Using a Generic Transfer Function in a Dual-Porosity Model

Flow in carbonate reservoirs is strongly influenced by fractures present in the geological formations. An accurate characterization of fracture flow is needed to forecast oil recovery and optimize production. We present a general dual-porosity model. It is based on an unstructured finite element - finite volume technique which solves the governing equations for two-phase flow fully implicitly. Mass transfer between fractures and matrix is computed with a generalized transfer function, the only known analytic solution for Darcy law with capillarity.

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MS32

An Analytical Approach to Green Oxidation

Oxidation, a process in which oxygen is added to break pollutants, often uses chemicals that can result in the production of hazardous substances. The main goal of the project is to be able to estimate the rates of the reactions based on experimental observations. We have developed perturbation techniques which allowed us to derive an approximate solution. It is expected that these techniques will yield even more far-reaching results when applied to more realistic systems.

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MS33

A Second Order Virtual Node Algorithm for Stokes Flow Problems with Interfacial Forces and Discontinuous Material Properties

We present a numerical method for the solution of the Stokes equations that handles interfacial discontinuities due to both singular forces and discontinuous fluid properties such as viscosity and density. The discretization couples a Lagrangian representation of the material interface with an Eulerian representation of the fluid velocity and pressure. The method is efficient, easy to implement and yields discretely divergence free velocities that are second-order accurate. Numerical results indicate second order accuracy for the velocities and first order accuracy for the pressure in l-infinity.

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MS33

A Fast Method for Interface and Parameter Estimation in Linear Elliptic PDEs with Piecewise Constant Coefficients

We present a new method for the recovery of the parameters and interface from an observed solution to embedded interface linear elliptic PDEs with piecewise constant coefficients. Our approach uses the linear nature of these equations to derive a function that is approximately equal to the coefficients across the entire domain. We recover the coefficients using split Bregman implementations of standard piecewise constant segmentation methods. We demonstrate the method on Poisson's equation and linear elasticity.

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MS33

Efficient Symmetric Positive Definite Second-Order Accurate Monolithic Solver for Fluid/Solid Interactions

We introduce a robust and efficient method to simulate strongly coupled (monolithic) fluid/rigid-body interactions. We take a fractional step approach, where the intermediate state variables of the fluid and of the solid are solved independently, before their interactions are enforced via a projection step. Overall, the computational time to solve the projection step is similar to the time needed to solve the standard fluid-only projection step. Numerical results indicate the method is second-order accurate in the l-infinity norm and demonstrate that its solutions agree quantitatively with experimental results.

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MS33

A Second Order Virtual Node Method for Elliptic Interface Problems with Interfaces and Irregular Domains in Three Dimensions

We present a numerical method for the variable coefficient Poisson equation in three-dimensional irregular domains with interfacial discontinuities. The discretization embeds the domain and interface into a uniform Cartesian grid augmented with virtual degrees of freedom to provide accurate treatment of jump and boundary conditions. . As in Bedrossian et al, this is used in a discontinuity removal technique that yields the standard 7-point stencil across the interface and only requires a modification to the right-hand side of the linear system.

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MS34

The Post-Fragmentation Density Function for Bacterial Aggregates

The post-fragmentation probability density of daughter flocs is one of the least understood aspects of modeling flocculation. A wide variety of functional forms have been used over the years to characterize fragmentation, and few have had experimental data to aid in its construction. In this talk, we discuss the use of 3D positional data of K. pneumoniae bacterial flocs in suspension to construct a probability density of floc volumes after a fragmentation event. Computational results are provided which predict that the primary fragmentation mechanism for medium to large flocs is erosion, as opposed to the binary fragmentation mechanism (i.e. a fragmentation that results in two similarly-sized daughter flocs) traditionally assumed.

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MS34

Modelling Cell Polarity: Theory to Experiments

In order to migrate, cells recruit various proteins to the plasma membrance and spatially segregate them to form a front and back. I present two possible mechanisms for this symmetry breaking process, and explain how cells can regulate the transition from a homogeneous, "resting cell", state to a spatially heterogeneous state corresponding to a polarized cell. I then focus on experimentally distinguishing between various proposed polarity models in crawling cells through perturbations of cell geometry.

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MS34

Epidemic Spread of Influenza Viruses: The Impact of Transient Populations on Disease Dynamics

Recent H1N1 pandemic and recent H5N1 outbreaks have brought increased attention to the study of the role of animal populations as reservoirs for pathogens that could invade human populations. Here we study the interactions between transient and resident bird populations and their role on dispersal and persistence. A meta-population framework based on a system of nonlinear ordinary differential equations is used to study the transmission dynamics and control of avian diseases. Epidemiological time scales and singular perturbation methods are used to reduce the dimensionality of the model. Our results show that mixing of bird populations (involving residents and migratory birds) play an important role on the patterns of disease spread.

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MS34

Modeling the Cofilin Pathway and Actin Dynamics in Cell Motility Activity of Mammary Carcinomas

Polymerization of actin cytoskeleton leads to cell migration, a vital part of normal physiology from embryonic development to wound healing. However, it also occurs in the pathological setting of cancer metastasis. Here I present mathematical models of actin regulation by cofilin which has been identified as a critical determinant of metastasis. I will discuss results obtained from simulations and steady state analysis and their biological implications, as well as modeling challenges that arise.

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MS35

Multiscale Simulation and Upscaling Multi-Species Reactive Transport from the Pore to Macro Scale

Abstract not available at time of publication.

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MS35

Multiscale Modeling and Simulation of Fluid Flows in Deformable Porous Media

A multiscale framework for fluid-structure interaction problems in inelastic media will be presented. Stokes flow is assumed at the pore scale with a general nonlinear elastic model for deformations. Due to complexity of pore-level interaction an iterative macroscopic model that consists of nonlinear Darcy equations and upscaled elasticity equations modeled via an iterative procedure is proposed. Numerical results for the case of linear elastic solid skeleton are presented for a number of model problems.

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MS35

Coupling Modeling for Compressible Fluid Flow in the Elastic Porous Media

In this work, we consider the dynamical response of a non-linear plate with viscous damping, perturbed in both vertical and axial directions interacting with a Darcy flow. We first study the problem for the non-linear elastic body with damping coefficient. We prove existence and uniqueness of the solution for the steady state plate problem. We investigate the stability of the dynamical non-linear plate problem under some condition on the applied loads. Then we explore the fluid structure interaction problem with a Darcy flow in porous media. In an appropriate Sobolev norm, we build an energy functional for the displacement field of the plate and the gradient pressure of the fluid flow. We show that for a class of boundary conditions the energy functional is bounded by the flux of mass through the inlet boundary.

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MS35

A Mixed Finite Element Framework for the Biot Model in Poroelasticity

Poroelasticity is the modeling of the time-dependent coupling between the deformation of porous materials and the fluid flow inside. It has been well-known that standard Galerkin finite element methods produce unstable and oscillatory numerical behavior of the pressure, which is known as *locking*. We present a mixed finite element formulation that has been designed to overcome locking. The formulation is based on coupling two mixed finite element formulations for the flow and mechanics problems. We discuss *a priori* error estimates and show some numerical results.

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MS36

Automatic Differentiation in Chebfun: Implementation and Usage

The implementation of Automatic Differentation (AD) in Chebfun is described. Whereas standard AD implementations compute Jacobians, Chebfun works in a continuous framework so the derivatives are Fréchet derivatives. The current implementation offers automatic linearity detection and linearisation of differential operators, as well as interior point and jump conditions in differential equations through AD of functionals. Examples of AD usage in Chebfun will be given.

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MS36

Spectral Deferred Correction in Chebfun for Time-dependent PDEs

Chebfun's goal of providing automatic, accurate results for 1D problems is challenging for time-dependent PDEs. Currently Chebfun uses a built-in stiff integrator of order 1-5. Huang et al. showed that spectral deferred correction can be generalized to a Krylov iteration for a spectrally computed error, preconditioned by low-order integration. This gives an A-stable, symplectic and reversible integration method capable of very high accuracy. It is readily implemented with Chebfun's discretization and automatic differentiation capabilities.

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MS36

An Overview of Differential Equations in Chebfun

Chebfun allows users to interact with functions in Matlab as if they were vectors, giving 'symbolic feel but numeric speed'. Chebops extend this functionality to operators and matrices, allowing a natural and efficient means of solving differential equations. In this introductory talk we'll open the chebop hood to take a look its core components, including the adaptive collocation and domain decomposition processes, and the enforcement of boundary conditions

through a new technique of rectangular projection.

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MS36
Computation of Frequency Responses of PDEs in Chebfun

We describe how frequency responses of PDEs with one spatial variable can be computed in Chebfun. Our method recasts the frequency response operator as a two point boundary value problem and it has two advantages over currently available schemes: first, it avoids numerical instabilities encountered in systems with differential operators of high order and, second, it alleviates difficulty in implementing boundary conditions. We provide examples from fluid dynamics to illustrate utility of the proposed method.

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MS37
Two Layer Model for Local Tear Film Dynamics

Many tear film models utilize a single-layer approach that represents only the aqueous layer, which constitutes the majority of the tear film. In such models, the layer is dominated by shear stresses. Some recent models have incorporated surfactant effects at the liquid-air interface to model the effects of polar lipids there. The model presented in this talk includes a thin lipid layer between the aqueous layer and the air, which is dominated by extensional flow. Our results show that the thin extensional layer significantly perturbs the aqueous layer flow.

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MS37
Defects and Heterogeneity in Liquid Coatings

Fluid coatings occur in situations from the manufacture of semiconductors to the foam lacing left behind after drinking a pint of beer. Sometimes coating uniformity is desirable, but in many cases, coatings are heterogeneous, with either defects or spontaneous or deliberate patterning. We examine the deposition of isolated bubbles in Landau–Levich (dip coating) flow of a pure liquid, and the self-assembly of particles in Landau–Levich flow of a suspension. These phenomena are explained through a combination of modeling, experiment, and analysis.

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MS37
Behavior of Droplets on a Thin Film

A drop of fluid on another fluid is modeled by a system of fourth order nonlinear PDE derived using the lubrication approximation. We assume the two fluids are Newtonian, incompressible, and immiscible. Relevant questions to this problem include: When does the drop spread over the underlying fluid? When does the drop touch the bottom surface? When does the drop break through the top interface? We explore these questions analytically, numerically, and experimentally.

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MS37
Fingering Instability Down the Outside of a Vertical Cylinder

We examine the fingering dynamics of a gravity-driven contact line of a thin viscous film traveling down the outside of a vertical cylinder of radius R. A lubrication model is derived for the film height in the limit that $H/R \ll 1$ (H is the upstream film height). Results from a linear stability analysis of the contact line are compared to experimental data. The influence of curvature will also be discussed.

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MS38
Networks, Communities and the Ground-Truth

The Web, society, information, cells and brain can all be represented and studied as complex networks of interactions. Nodes in such networks tend to organize into clusters and communities, which represent the fundamental structures for understanding the organization of complex systems. Even though detection of network communities is of significant importance for computer science, sociology and biology, our understanding of the community structure of large networks remains limited. We study a set of more than 200 large networks with the goal to understand and identify communities in networks. We challenge the conventional view of network community structure and show that it is not exhibited by the large real-world networks. We then present a new conceptual model of network community structure, which reliably captures the overall structure of networks and accurately identifies the overlapping nature of network communities.

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MS38
High-Performance Metagenomic Data Clustering and Assembly

We present a novel de Bruijn graph-based parallel assembly approach for assembling metagenomic reads. The assembler employs a maximum-likelihood framework that handles the challenges posed by increased polymorphism and over-representation of conserved regions. It also provides tolerance for errors due to the incomplete and fragmentary nature of the reads. We also propose a two-way, multi-species, multi-dimensional Poisson mixture model-based method for representing reads from a metagenome. We use this method to cluster metagenomic reads by their species of origin, and to characterize the abundance of each species.

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MS38

Influence Propagation on Large Graphs

Given a network of who-contacts-whom, will a contagious virus/product/meme take-over (cause an epidemic) or die-out quickly? What will change if nodes have partial, temporary or permanent immunity? What if the underlying network changes over time (e.g., people have different connections during the day at work, and during the night at home)? Propagation style processes can model well many real-world scenarios like epidemiology and public health, information diffusion etc. We present results on understanding the tipping-point behavior of epidemics (enabling among other things faster simulations), predicting who-wins among competing viruses, and developing effective algorithms for immunization and marketing for several large-scale real-world settings. Finally, we collected and analyzed Twitter data over multiple months, to understand the role of external effects in how different hashtags (topics) spread. We showed fundamental differences in the dynamics of hashtags e.g. we found that hashtags of a political nature are primarily driven by outside influences, even though many people may be tweeting about them.

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MS38

Scaling Graph Computations at Facebook

With more than 800 million active users and 68 billion edges, scalability is at the forefront of concerns when dealing with the Facebook social graph. This talk will discuss two recent advances. First, through the development of a novel graph sharding algorithm for load-balancing graph computations, we were able to reduce the query time of a realtime system by 50%. Second, when computing the average graph distance between users on Facebook, empirical advances in the compression of the Facebook graph was a key step in speeding up the computation.

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MS39

Optimization-Based Decomposition of Multiphysics Problems with Applications

We present a new, optimization-based framework for computational modeling. The framework uses optimization and control ideas to assemble and decompose multiphysics operators and to preserve their fundamental physical properties in the discretization process. Our approach relies on three essential steps: decomposition of the original problem into subproblems for which discretizations and robust solvers are available; integration of the subproblems into an equivalent constrained optimization problem; and solution of the resulting optimization problem either directly as a fully coupled algebraic system, or in the null space of the constraints.

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MS39

Blended Force-based Quasicontinuum Methods

The development of consistent and stable quasicontinuum models for multi-dimensional crystalline solids remains a challenge. For example, proving stability of the force-based quasicontinuum (QCF) model remains an open problem. In 1D and 2D, we show that by blending atomistic and Cauchy–Born continuum forces (instead of a sharp transition as in the QCF method) one obtains positive-definite blended force-based quasicontinuum models if and only if the width of the blending region scales as $O(N^{1/5})$ atomic lattice spacings (or the width scales as $O(N^{-4/5})$ in the macroscopic scale). We present computational results and analysis.

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MS39

Energy-Based A/C Coupling for Pair Interaction

I will present a recent development in construction and analysis of an energy-based atomistic-to-continuum coupling for two-body interaction (limited to zero-temperature statics of simple crystals).

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MS39

Blended Energy-based Quasicontinuum Methods

We present the energy-based blended quasicontinuum (BQCE) method for coupling atomistic and continuum models. We give error estimates for BQCE for 3D and multi-lattice crystals, and we give optimal choices of the approximation parameters (the blending function and finite element mesh) for the problem of a localized defect surrounded by a perfect crystal. Our formulation of BQCE for multi-lattice crystals uses a novel continuum model which we also discuss. Finally, we give numerical experiments which confirm the predictions of our error estimates.

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MS40

Numerical Algebraic Geometry via Macaulay's Perspective

F.S. Macaulay regarded theoretical solutions as preliminary, a final solution to a problem is one which can actually be computed. The methods he proposed in his famous 1916 book are therefore computational but not all feasible at that time. This talk will outline the speaker's adaptation of Macaulay's methods, including H-bases and inverse arrays, using modern numerical linear algebra. Examples involving the functorality of the global dual will be given.

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MS40

Preconditioning with H-Bases Computed Using Dual Space Operations

When solving polynomial systems using homotopy continuation, it is sometimes the case that we end up with a large number of paths going to ∞. We want to precondition these systems using H-bases in order to remove paths going to ∞. We calculate the H-bases numerically from operations on the dual space. When we dualize again, we recover H-bases with the same variety as the original ideal. This process removes the extraneous pieces at ∞ with at most an addition of "junk" points. This eliminates paths going to ∞ in the homotopy continuation run.

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MS40

Elimination of Pseudo-components in Numerical Primary Decomposition

The goal of a numerical primary decomposition algorithm is to produce an approximation to a general point on each component of a scheme defined by an ideal of polynomials with complex coefficients. Our approach based on homotopy continuation and the concept of a deflated variety produces extraneous, the so-called pseudo-, components. This talk will outline an algorithm to detect these using approximate Macaulay dual space computation.

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MS40

Extended Precision Path Tracking in Parallel

To compensate for the overhead of extended precision (in particular: of double double and quad double arithmetic), we investigated the use of multiple cores on regular processors and general purpose graphics processing units. Because the cost of evaluating and differentiating polynomials often dominates the computational work in path tracking, we developed and implemented multithreaded algorithms on multicore processors and massively parallel algorithms for general purpose GPUs for multivariate polynomial evaluation and differentiation.

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MS41

A Nonconforming Finite Element Method for an Acoustic Fluid-Structure Interaction Problem

In this work, we propose and analyze a nonconforming finite element approximation of the vibration modes of acoustic fluid-structure interaction. The numerical scheme is based on the irrotational fluid displacement formulation which eliminates the occurence of spurious eigenmodes. Our method uses weakly continuous P1 vector fields for the fluid and classical piecewise linear elements for the fluid. On properly graded meshes, we show optimal order error estimates which are validated by numerical experiments.

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MS41

Fluid-fluid Calculations using the Evolve-filter-relax Regularization Strategy

Calculations for a model of two fluids coupled across a shared interface are performed by using the evolve, then filter and relax method, motivated by atmosphere-ocean interaction. This method has a regularization effect and is computationally attractive since the evolution, filtering and relaxation steps can be decoupled. Different relaxation parameters are appropriate for the two fluids. An algorithm is described to determine these parameters automatically at each time step to improve model accuracy.

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MS41

Large Eddy Simulation of the Quasi-Geostrophic Equations of Oceanic Flows

We developed an approximate deconvolution (AD) LES model for the two-layer quasi-geostrophic equations(QGE). The AD closure modeling approach is appealing for geophysical flows because it needs no additional phenomenological approximations to the original equations, and it can achieve high accuracy by employing repeated (computationally efficient and easy to implement) filtering. We applied the AD-LES model to mid-latitude two-layer square oceanic basins, which are standard prototypes of stratified ocean dynamics models. Compared with a high-resolution simulation, AD-LES yielded accurate results at significantly lower computational cost. The sensitivity of the AD-LES results with respect to changes in input parameters was also performed. We discovered that although the AD-LES model was robust with respect to changes in parameters, changing the spatial filter made a huge difference. Two spatial filters were investigated in the AD-LES model: tridiagonal and elliptic differential. We found the tridiagonal filter did not introduce any numerical dissipation in the AD-LES model. The differential filter, however, added a significant amount, and our numerical results show the new AD-LES model used in with the differential filter can be employed successfully on meshes significantly coarser than the Munk scale and with an eddy viscosity coefficient that is dramatically lower than that used in the original two-layer QGE. Although we do not provide a solution to the longstanding quest for finding a rigorous derivation of the eddy viscosity coefficients used in ocean modeling, we put forth a novel approach, serendipitously discovered in our numerical investigation. The main strength of this new approach is that the modeling error can be disentangled from the numerical discretization error and can be studied separately in this framework. This could lead to more robust and general LES models for large scale geophysical flows.

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MS41

Uncertainly Quantification for PDEs

Abstract not available at time of publication.

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MS42

Improving Earthquake Ground Motion Estimates with Blue Gene/Q

This project aims to produce the first state-wide physics-based probabilistic seismic hazard analysis (PSHA) map for California, a goal only feasible with petascale computing. The relevant phenomena span many orders of magnitude in spatial scale, requiring high-resolution simulations. Furthermore, proper uncertainty estimation for PSHA requires simulations of large numbers of possible events. We will discuss the necessary optimizations to our finite-element simulation codes for the Blue Gene/Q architeture.

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MS42

Blue Gene/Q Architecture and Programming Models

Managing the million-way concurrency found in the Blue Gene/Q architecture requires new thinking about algorithms and programming models. This talk will describe the hardware architecture in detail and the connection to hybrid (i.e. multithreaded) programming models. Performance of fundamental operations will be measured using benchmarks derived from real applications.

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MS42

Chemical Applications of the Multiresolution Adaptive Numerical Environment for Scientific Simulation (MADNESS)

MADNESS (multiresolution adaptive numerical environment for scientific simulation) is a general numerical framework to solve integral and differential equations in multiple dimensions. With its parallel runtime and numerical methods, MADNESS has proven to be a robust platform for discretized problems, in particular those found in quantum chemistry, nuclear physics, solid-state physics, atomic and molecular physics. In this work we will discuss asynchronous parallelism model implemented in a multi-threaded scheme and its application to energy storage and conversion using linear-response density-functional theory.

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MS42

Accelerating and Benchmarking GAMESS on BlueGene/Q

General Atomic and Molecular Electronic Structure System (GAMESS) is a popular *ab-initio* quantum chemistry program. The Fragment Molecular Orbital (FMO) method implemented in GAMESS is highly-scalable and allows one to perform highly accurate calculations on very large molecular systems. We will describe our experience porting and optimizing GAMESS for Blue Gene/Q. The algorithm used to multithread the integral kernels in GAMESS to take full advantage of the hardware capabilities of Blue Gene/Q will be discussed in detail. Lastly, we will present several benchmark results, including FMO calculations on water clusters.

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MS43

An Analytical Level Set Method for Eigenvalue Shape Optimization Problems

We propose an eigenvalue shape optimization method based on representing the boundary of the domain as the zero level set of a linear combination of eigenfunctions corresponding to the same eigenvalue. The optimal shape is discovered by adjusting the shared eigenvalue and the coefficients of the linear combination. The method works in any number of dimensions and is characterized by utmost simplicity, arbitrarily high accuracy for a broad range of problems, as well as the ability to produce an exact analytical solution for an approximate problem.

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MS43

Shape Recognition Based on Eigenvalues of the Laplacian

Recently, there has been a surge in the use of the eigenvalues of linear operators in problems of pattern recognition. In this presentation, we discuss theoretical, numerical, and experimental aspects of using four well known linear operators and their eigenvalues for shape recognition. In particular, the eigenvalues of the Laplacian operator under Dirichlet and Neumann boundary conditions, as well as those of the clamped plate and buckling of a clamped plate are examined. Since the ratios of eigenvalues for each of these operators are translation, rotation and scale invariant, four feature vectors are extracted for the purpose of shape recognition. These feature vectors are then fed into a basic neural network for training and measuring the performance of each of the feature vectors which in turn were all shown to be reliable features for shape recognition. The presentation focuses on finite difference schemes for these operators and summarizes key facts about their eigenvalues that are of relevance in image recognition. (*) Joint work with M. B. H. Rhouma and M. A. Khabou.

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MS43

Shape Optimization with the Vector Maxwell Equations

An intuitive framework is presented for shape optimization with the vector Maxwell equations. Through adjoint techniques, two simulations per iteration give both the shape and topological derivatives. The method is applied to the design of a sub-wavelength solar cell texture, resulting in the highest reported absorption enhancement factor for high-index, thin-film media. The enhancement is achieved by shaping the bandstructure and optimizing the in-coupling, possible only through non-intuitive, higher-order Fourier coefficients.

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MS43

Characterization of Weighted Graphs using Graph Laplacians

We will discuss our recent effort on characterizing and clustering weighted graphs using their morphological features extracted by spectra of their graph Laplacians. Compared to unweighted graphs (which we studied them previously), the graphs with weights pose a further challenge both in theory and practice. We will also discuss the eigenfunction concentration phenomenon on a class of simple trees where such a phenomenon does not occur if unweighted.

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MS45

A Treecode Algorithm for N-body Interactions with Disjoint Source and Target Particles

Energy and force computations are usually the bottleneck in molecular dynamics and Monte-Carlo simulations. Most algorithms for speeding up the N-body interactions are for a set of particles interacting with itself. We will present a treecode algorithm that offers considerable speed up for (1) a set of particles interacting with itself as well as (2) interactions between a disjoint pair of source and target particles while achieving high accuracy.

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MS45

Multi-frequency Iterative Integral Equations Method for the Shape Reconstruction of an Acoustically Sound-soft Obstacle Using Backscattering

We present a method of solving the problem of obtaining a reconstruction of a planar acoustically sound-soft obstacle from the measured far-field pattern generated by plane waves with a fixed incidence and varying frequencies. We solve iteratively the problem for each frequency, from the lowest to the highest, using as an initial guess the solution given by the previous frequency. We present numerical results showing the benefits of our approach.

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MS45

A Novel Multiscale Model of Glioblastoma Multiforme (gbm)

Glioblastoma multiforme (GBM) is the most malignant, invasive, and lethal form of brain cancer; the median survival time of patients diagnosed with GBM is 15 months. We develop an adaptive, multiscale mathematical and numerical model to study the development of GBM. We use a continuum (partial differential equation) model to describe the changes in the concentrations of important chemicals and proteins, such as glucose, oxygen, TGF_{α}, PLC_{γ}, and an agent-based model for the tumor cells. In the development of a tumor, distinct regions evolve. There is eventually a necrotic core filled with dead cells surrounded by a region of quiescent (inactive) cells. The quiescent region is rimmed by proliferating and/or migrating cells. While one may acceptably describe the quiescent or necrotic regions of the tumor with a continuum model which would represent activities on a macroscale, such a model would not capture the important details in the invasive regions where the cells are actively migrating and dividing. A fully microscale model would represent each cell as an individual entity but since a fully grown tumor has 10^{12} cells, this approach is too computationally expensive. We develop a numerical model on adaptive quadtree grids that allows for multiresolution. A *phenotypic function* determines the phenotype population in each grid block as a function of the concentration of chemicals and proteins there, and cues changes in the grid resolution periodically to accurately capture the tumor structure.

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MS45

Improving Hurricane Storm Surge Forecasting using Data Assimilation Methods

Uncertainty is inherent in numerical forecast models as well as in measurements of model solutions. Given both a model and measurements, advanced data assimilation methods can be used to improve state estimates of nonlinear problems. One such method, the singular evolutive interpolated Kalman (SEIK) filter, has been applied to the Advanced Circulation (ADCIRC) storm surge model. Here ADCIRC along with data produced from a detailed hindcast study is used to improve hurricane storm surge forecasts.

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MS46

Orbits of Projective Point Configurations

Given an $r \times n$ matrix, thought of as representing n points in projective $(r-1)$-space, we consider the closure of the orbit of all projectively equivalent matrices. I will discuss the equations cutting out this variety, its finely graded Hilbert series, and their relation to the matroid of the point configuration.

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MS46

Finiteness Theorems and Algorithms for Polynomial Equations in an Infinite Number of Variables

We discuss the theory of symmetric Groebner bases, a concept allowing one to prove Noetherianity results for symmetric ideals in polynomial rings with an infinite number of variables. We also explain applications of these objects to other fields such as algebraic statistics, and we present an algorithm for computing with them on a computer. Some of this is joint work with Matthias Aschenbrener and Seth Sullivant.

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MS46

Stable Intersections of Ttropical Varieties

Taking the stable intersection of a list of tropical hypersurfaces is a purely combinatorial operation. The stable intersection can also be obtained by generically perturbing the coefficients of the defining equations and taking the tropical variety of the ideal they generate. This observation leads to a new proof of Bernstein's theorem. We discuss how some combinatorial properties of stable intersections can be proven either purely combinatorially or be derived from tropical varieties of ideals.

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MS46

Computer-aided Design Algebra and Combinatorics

Computer Aided Design (CAD) software allows a user to specify a finite number of rigid bodies and pairwise **c**oincidence, **a**ngular, and **d**istance (cad) constraints among them. It is important to know when such a "body-and-cad" framework is rigid or when the bodies may move relative to one another while maintaining the given constraints. A body-and-cad framework may be specified by an edge-colored multigraph. I will discuss a combinatorial characterization of the rigidity of a body-and-cad framework in which 20 of the 21 possible 3D constraints may appear. For our analysis we build on algebro-geometric methods developed by White and Whiteley to study the rigidity of systems consisting of a finite collection of bodies connected by fixed-length bars using flexible joints.

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MS47

A Global Holmgren Theorem for Hyperbolic PDE

A global uniqueness theorem for solutions to hyperbolic differential equations with analytic coefficients in a space-time cylinder $Q = (0,T) \times \Omega$ is established. Zero Cauchy data on a part of the lateral C^1-boundary will force every solution to a homogeneous hyperbolic PDE or system to vanish at half time $T/2$ provided that $T > T_0$. The minimal time T_0 depends on the geometry of the slowness surface of the hyperbolic operator. This theorem is an extension of an earlier result by Walter Littman from 2000. Furthermore, it is shown that this global uniqueness result holds for hyperbolic operators with C^1-coefficients as long as they satisfy the conclusion of Holmgren's Theorem.

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MS47

Conservation Laws in Mathematical Biology

In this talk I will consider conservation laws for a system of hyperbolic equations, in which the coefficients are nonlinear and nonlocal functions of unknown variables. I will explain how each such system arises as a mathematical model of a biological process, and address the mathematical results and, in some cases, open problems associated with the model equations. The examples are taken from the the areas of public health (drug resistance strains of bacteria), immune cell (Th cell differentiation), movement of molecules along axon, cancer, and wound healing

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MS47

Controllability and Regularity of Some 1-d Elastic Systems with Internal Point Masses

In the case of a wave equation with an internal point mass, it is known that exact controllability holds on an asymmetric space, where the regularity is higher on one side of the mass. We consider several variations of this problem, including the SCOLE beam model, but with an interior rigid body and thermoelastic systems with internal masses.

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MS47

Some Absolutely Continuos Schrödinger Operators With Oscillating Potentials

In this talk we report on the principle of limiting absorption for a family of Schrödinger operators of the form

$$-\Delta + c \sin b|x|^\alpha / |x|^\beta.$$

More specifically, we formulate conditions on the parameters c, b, α, β and interval $\mathcal{I}$ which ensure that the PLA holds for such an operator over the interval $\mathcal{I}$. Note that although this potential is spherically symmetric, the validity of the PLA for the seperated operator does not imply the PLA for the original operator. Our principal reference is the forthcoing paper of Golennia and Jecko, A New Look At Mourre's Commutator Theory.

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MS48

Modeling Evaporation and Transport in Porous Media. Comparing Models Using Different Dependent Variables

Fick's law for molecular diffusion can be used to describe how water vapor is transported through a gas mixture. The general forms of Fick's law can be written using gradients of either mass concentration, mole fraction, or chemical potential of the water vapor as dependent variables. Using concentration as a dependent variable is more natural for the modeling process (as it appears naturally in the conservation of mass equations), but can yield unnatural boundary conditions and nonlinear equations. Using chemical potential is less natural for modeling but yields governing equations that are more mathematically tractable and boundary conditions that are more natural. In this talk we consider evaporation and diffusion of water vapor. Depending on the choice of dependent variable we derive different sets of governing equations for the transport of water vapor. A careful derivation and analysis of each model will be presented for water evaporation and diffusion in a simple capillary tube, and comparisons of evaporation rates will be made between the models. Consequences for macroscale modeling will be discussed.

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MS48
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS48
Numerical Methods for Shallow Water Models

In this talk we will introduce and discuss numerical schemes for the shallow water equations. These equations are widely used in many scientific applications related to modeling of water flows in rivers, lakes and coastal areas. Furthermore, many real world engineering applications require the use of triangular meshes due to the complicated structure of the computational domains of the problems being investigated. Therefore the development of robust and accurate numerical methods for the simulation of shallow water models is important and challenging problem. In our talk we will discuss the recently developed numerical schemes for such models. We will demonstrate the performance of the proposed methods in a number of numerical examples.

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MS48
A Comparison of Finite Element Methods for Strongly Density Dependent Flows

Saltwater intrusion is a frequent issue in coastal freshwater aquifers. We develop a Discontinuous Galerkin (DG) formulation for these saltwater flow and transport problems. The transport scheme must handle sharp fronts while the flow scheme requries high accuracy. DG methods have potential advantages over continuous Galerkin models for such problems. We discretize the flow with local DG and the transport with Non-symmetric, Interior Penalty Galerkin. We present the formulation and comparisons for saltwater intrusion benchmarks.

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MS49
Delaying Wetting Failure In Coating Flows Via Meniscus Confinement

Wetting failure brought about by air entrainment remains one of the biggest obstacles to faster operation of numerous processes that deposit coatings of thin liquid films. Improving upon the coating speeds used in current technologies requires a better understanding of how system parameters influence wetting failure. We use both experiment and modeling to determine the effect of one such parameter—meniscus confinement—on the initiation of dynamic wetting failure. Our experimental apparatus consists of a scraped steel roll that rotates into a bath of glycerol, and confinement is imposed via a gap formed between a coating die and the roll surface. Comparison of the data from confined and unconfined systems—obtained via flow visualization—shows a clear increase in the relative critical speed as the meniscus becomes more confined. A hydrodynamic model for wetting failure is developed and analyzed with (i) lubrication theory and (ii) a two-dimensional finite element method (FEM). Both approaches do a remarkable job of matching the observed confinement trend, but only the two-dimensional model yields accurate estimates of the absolute values of the critical speeds due to the highly two-dimensional nature of the stress field in the displacing liquid. The overall success of the hydrodynamic model suggests a wetting failure mechanism primarily related to viscous bending of the meniscus.

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MS49
Tear Film Dynamics on an Eye Shaped Domain

We consider a tear film dynamics model on a 2-D eye shaped domain with specification of the flux normal to the boundary. The domain is fixed in time, but we cycle the time dependence of the flux boundary condition. This treatment is a drastic simplification of what occurs *in vivo*. Model simulations are conducted in the OVERTURE computational frame work. Results are compared with existing tear film models with both 1-D and 2-D domains as well as clinical measured data.

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MS49

Tear Film Dynamics with Surfactant Transport and Osmolarity

We consider a model problem for the breakup up of the tear film including surface tension, Marangoni stresses, insoluble surfactant transport, evaporation, osmolarity transport, osmosis and wetting of corneal surface. Surface-concentration evaporation mimics the tear film lipid. In many, the Marangoni effect seems to eliminate a localized area of increased evaporation while the osmolarity increases because of evaporation.

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MS49

Effective Slip for An Upper Convected Maxwell Fluid

We consider an upper convected Maxwell fluid with solvent and diffusion undergoing shear flow at a solid wall. We show that even for this simple model, stress diffusion may lead to plug flow and sharp boundary layers near the solid wall. We discuss this for a simple channel flow configuration and generalize the results to lubrication models of a thin film flowing over a solid substrate. For this free boundary problem a distinguished limit can be identified. The lubrication models are found to correspond in part to previously known lubrication models with a slip boundary condition.

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MS50

Exploiting Saliency in Compressive and Adaptive Sensing

Recent developments in compressive and adaptive sensing have demonstrated the tremendous improvements in sensing resource efficiency that can be achieved by exploiting sparsity in high-dimensional inference tasks. In this talk we describe how compressive sensing techniques can be extended to exploit saliency. We discuss our recent work quantifying the effectiveness of a compressive sensing strategy that accurately identifies salient features from compressive measurements, and we demonstrate the performance of this technique in a two-stage active compressive imaging approach to automated surveillance.

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MS50

Sharp Recovery Bounds for Convex Deconvolution, With Applications

This work investigates the limits of a convex optimization procedure for the deconvolution of structured signals. The geometry of the convex program leads to a precise, yet intuitive, characterization of successful deconvolution. Coupling this geometric picture with a random model reveals sharp thresholds for success, and failure, of the deconvolution procedure. These generic results are applicable to a wide variety of problems. This work considers deconvolving two sparse vectors, analyzes a spread-spectrum coding scheme for impulsive noise, and shows when it is possible to deconvolve a low-rank matrix corrupted with a special type of noise. As an additional benefit, this analysis recovers, and extends, known weak and strong thresholds for the basis pursuit problem.

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MS50

Fast Global Convergence of Gradient Methods for High-dimensional Statistical Recovery

Many statistical M-estimators are based on convex optimization problems formed by the combination of a data-dependent loss function with a norm-based regularizer. We analyze the convergence rates of projected gradient methods for solving such problems, working within a high-dimensional framework that allows the data dimension d to grow with (and possibly exceed) the sample size n. This high-dimensional structure precludes the usual global assumptions—namely, strong convexity and smoothness conditions—that underlie much of classical optimization analysis. We define appropriately restricted versions of these conditions, and show that they are satisfied with high probability for various statistical models. Under these conditions, our theory guarantees that projected gradient descent has a globally geometric rate of convergence up to the *statistical precision* of the model, meaning the typical distance between the true unknown parameter θ^* and an optimal solution $\hat{\theta}$. This result is substantially sharper than previous convergence results, which yielded sublinear convergence, or linear convergence only up to the noise level. Our analysis applies to a wide range of M-estimators and statistical models, including sparse linear regression using Lasso (ℓ_1-regularized regression); group Lasso for block sparsity; log-linear models with regularization; low-rank matrix recovery using nuclear norm regularization; and matrix decomposition. This is based on joint work with Alekh Agarwal and Martin Wainwright.

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MS50

Robust Image Recovery via Total Variation Minimization

Discrete images, consisting of slowly-varying pixel values except across edges, have sparse or compressible representations with respect to the discrete gradient. Despite being a primary motivation for compressed sensing, stability results for total-variation minimization do not follow directly from the standard "l1" theory of compressed sensing. In this talk, we present near-optimal reconstruction guarantees for total-variation minimization and discuss several related open problems.

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MS51

Version 2.0 of the Parallel Boost Graph Library: Message-Driven Solutions to Data-Driven Problems

Data-driven applications, such as graph analytics, are unique in that the computational structure of the applications is entirely dependent on the input data. This fact makes static analysis difficult and necessitates dynamic, lightweight, execution-time solutions. Version 2.0 of the Parallel Boost Graph Library (PBGL) demonstrates one approach to building a modular, scalable, and perhaps most importantly, performance portable set of graph kernels. The PBGL 2.0 uses the AM++ active messaging library (an implementation of the Active Pebbles programming and execution model) to provide portable, generic, thread-safe messaging support on a variety of platforms. On top of AM++, PBGL 2.0 provides a variety of graph types, auxiliary data structures, and algorithmic kernels suitable for both shared- and distributed-memory parallelism (e.g. threads and processes) with the potential for straightforward extension to various types of accelerators.

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MS51

Massive Graphs: The Way Forward

Large graph analytics have become an increasingly important in a wide variety of application areas such as internet search, bioinformatics, social media, and cybersecurity. Massive graphs push the state of the art in both big compute and big data. This presentation will collect and present the outstanding questions in this field that have been raised over the course of the mini-symposium.

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MS51

Extended Sparse Matrices as Tools for Graph Computation

Sparse matrices frame a powerful graph computation architecture. Extensions such as complex elemental types, runtime filtering and arbitrary semiring operations greatly expand the utility of sparse matrices for graph analytics. Implementations must also match available hardware to be useful. Individual shared-memory machines, distributed-memory clusters and cloud HPC systems all raise unique challenges, but significant commonality remains among them. This talk will cover how we address these challenges in our Knowledge Discovery Toolbox.

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MS51

Graph Analytics for Subject-Matter Experts: Balancing Standards, Simplicity, and Complexity

Subject-matter experts needing to analyze large graphs ideally want the abilities to incorporate data from disparate sources, perform simple analyses to find data needing deeper analysis, and execute complex analyses on that data, all via clear, reliable, and widely-available interfaces. Knowledge Discovery Toolkit (KDT) enables complex analyses on very large data (beyond what will reside in the memory of a single cluster node) through procedural interfaces, though it does not (yet) ingest numerous data formats. Emerging semantic-web technologies are starting to deliver the promise of straightforward fusing of disparate data sources through standard interfaces and ontologies, yet the current SPARQL 1.1 language does not support the calculation of complex graph metrics, such as betweenness centrality. This talk will cover our work to merge the ease-of-use of the semantic-web technologies with the complex analytics of KDT.

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MS52

Pointwise Estimates for Stokes Equation

In this talk I will describe new stability results of the finite element solution for the Stokes system in W^1_∞ norm on general convex polyhedral domain. In contrast to previously known results, W^2_r regularity for $r > 3$, which does not hold for a general convex polyhedral domains, is not required. I will briefly describe the main ideas of the proof that uses recently available sharp Holder pointwise estimates of the corresponding Greens matrix together with novel local energy error estimates, which do not involve an error of the pressure in a weaker norm.

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MS52

Conforming and Divergence Free Stokes Elements

We present a family of conforming finite elements for the Stokes problem on triangular meshes. We show that the elements satisfy the inf-sup condition and converge optimally. Moreover, the pressure space is exactly the divergence of the velocity space. Therefore the discretely divergence free functions are divergence free pointwise. We also show how the elements are related to a class of C^1 elements through the use of a discrete de Rham complex.

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MS52

Transparent Boundary Conditions and the Gap Condition for Stokes Elements

In the context of a Finite Element discretization of the Stokes equation, a gap property is the possibility of uniformly approximating velocities with discrete zero divergence by exactly solenoidal fields. This property seems to be rare among non-divergence-free stable Finite Element spaces for the Stokes equation. We will discuss it for some examples and we will prove that it implies the discrete well posedness of the simplest FEM-BEM coupled schemes for Stokes.

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MS53

Optimal Bilaplacian Eigenvalues

We consider the shape optimization for the clamped plate and buckling plate eigenvalue problems. We develop a numerical method using Hadamard's shape derivative and the Method of Fundamental Solutions as forward solver which allows to propose numerical candidates to be minimizers of the first ten eigenvalues of both problems.

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MS53

Principal Eigenvalue Minimization for an Elliptic Problem with Indefinite Weight

An efficient rearrangement algorithm based on Rayleigh quotient and rearrangement is introduced to the minimization of the positive principal eigenvalue under the constraint that the absolute value of the weight is bounded and the total weight is a fixed negative constant. Biologically, this minimization problem is motivated by the question of determining the optimal spatial arrangement of favorable and unfavorable regions for a species to survive. The optimal results are explored both theoretically and numerically.

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MS53

Microcavity Optimization via the Frequency-averaged Local Density of States

Applications such as lasers and nonlinear devices require optical microcavities with long lifetimes Q and small modal volumes V. We formulate and solve a full 3d optimization scheme, over all possible 2d-lithography patterns in a thin dielectric film. The key to our formulation is a frequency-averaged local density of states, where the frequency averaging corresponds to the desired bandwidth, evaluated by a novel technique: solving a single scattering problem at a complex frequency.

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MS55

Tracing the Progression of Retinitis Pigmentosa via Photoreceptor Interactions

Retinitis pigmentosa (RP) is a group of inherited degenerative eye diseases characterized by mutations in the genetic structure of the photoreceptors that leads to the premature death of the photoreceptors. We trace the progression of RP to complete blindness through each subtype via bifurcation theory. We show that the evolution of RP requires the failure of multiple components and that a delicate balance between nutrients and the rates of shedding and renewal is needed to halt its progression.

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MS55

Oscillation Criteria for Nonlinear Dynamic Equations

In this talk we consider the second-order linear delay dynamic equation

$$\left(p(t)y^{\Delta}(t)\right)^{\Delta} + q(t)y(\tau(t)) = 0$$

on a time scale T. By employing the Riccati transformation technique, we establish some sufficient conditions which ensure that every solution oscillates. The obtained results unify the oscillation of second-order delay differential and difference equations. We illustrate our results with examples.

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MS55

Order of Events and Optimal Control in Discrete Time Biological Models

The order of events in models with discrete time is crucial. Two examples illustrate the effect of the order of events on optimal control of models with discrete time. One example involves augmentation of an endangered species and the other example is a harvesting problem for an integrodifference population model.

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MS55

A Mathematical Modeling Approach to the Reversal of Type 2 Diabetes and β-Cell Compensation

Mathematically we explore fat accumulation and β-cell function in the progression of Type 2 diabetes (T2D). Extending previous models we consider a link between adipose tissue and insulin sensitivity. Incorporating fat and direct effects of both insulin and β-cell sensitivity, the latter embodies a logistic response. Qualitative description on glucose-insulin-β-cell, and fat dynamics with bifurcation analysis address irreversibility of T2D and β-cell failure which yield insight on clinical interventions targeted to certain stages of T2D.

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MS56

Jet Flows in Active Nematic Fluids

We have investigated the organisation, order and flow induced in an active fluid, consisting of an isotropic fluid containing elongated swimming organisms. Using an adapted form of the Ericksen-Leslie theory of liquid crystals, we have found instabilities from the trivial no-flow solution, which lead to kink-like flow profiles and flow-aligned orientational structures. There are also other, jet-like, solutions which are often higher energy solutions but are, at least locally, stable.

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MS56

Analysis of Smectic C* Films with Defects

We analyze a model for the elastic energy of planer c-director patterns in a smectic film. Because of boundary conditions and polar fields topological defects form in these patterns. We use a Ginzburg Landau model that allows the director field to have variable length and to vanish at the defect cores. We prove that if the models G-L parameter is small then low energy states develop degree +(-) one defects that tend to a minimal energy configuration with a limiting far field texture. Our main contribution is that we are able to treat the case of unequal splay and bend elasticity constants. Earlier analytic work for the G-L functional had been limited to the equal constant case.

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MS56

Shear Flow in Smectic A Liquid Crystals

The onset of a dynamic instability in the shear flow of planar aligned smectic A liquid crystals will be discussed. Oscillatory shear will also be examined and the results will be linked to the onset of an analogous dynamic instability for lipid bilayers induced by forced oscillations. Mathematical modelling equivalences will be highlighted and key critical control parameters will be identified for the occurrence of instabilities.

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MS56

Anisotropic Wave Propagation in Nematic Liquid Crystals

As early as 1972, Mullen, Luthi and Stephen [1] showed experimentally that the director alignment of a nematic liquid crystal induces an anisotropic propagation of acoustic waves. By contrast, Selinger and co-workers [2] have studied a liquid crystal cell where the nematic molecules can be realigned by an ultrasonic wave, leading to a change in the optical transmission through the cell. The existing models for this acousto-optic effect [2,3] propose a free energy that depends on the density gradient thus describing the nematic liquid crystal as a compressible second grade fluid. In the presentation I will show how the introduction in the stress tensor of the simple anisotropic term $\mathbf{n} \otimes \mathbf{n}$, $\mathbf{n}$

being the director field, easily reproduces the experimental anisotropic behaviour of the sound speed, thus providing a simpler first-grade model for the acousto-optic effect. It is worth noticing that Ericksen already considered this term in his seminal papers but subsequently it has been neglected. This term is non-hyperelastic. However, we show that it can be interpreted as the linear approximation of a new interaction term in the free energy for the NLC medium which couples the director field with the elastic properties of the fluid. Some noticeable consequences of this choice are then discussed.

[1] M.E. Mullen, B. Luthi and M.J. Stephen, "Sound velocity in a nematic liquid crystal", Phys. Rev. Lett. 28, 799-801 (1972).
[2] J.V. Selinger, M.S. Spector, V.A. Greanya, B.T. Weslowski, D.K. Shenoy, and R. Shashidhar, "Acoustic realignment of nematic liquid crystals", Phys. Rev. E 66, 051708 (2002).
[3] E.G. Virga, "Variational theory for nematoacoustics", Phys. Rev. E 80, 031705 (2009).

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MS57

Quasistatic Nonlinear Viscoelasticity and Gradient Flows

We consider the equation of motion for one-dimensional nonlinear viscoelasticity of strain-rate type under the assumption that the stored-energy function is λ-convex, allowing for solid phase transformations. We show how this problem can be formulated as a gradient flow, leading to existence and uniqueness of solutions. By approximating general initial data by those in which the deformation gradient takes only finitely many values, we show that the deformation gradient is instantaneously bounded and bounded away from zero. Finally, we discuss the open problem of showing that every solution converges to an equilibrium solution as time $t \to \infty$, proving by means of a new argument that this occurs in some previously unsolved cases.

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MS57

Energy Scaling Laws for Conically Constrained Thin Elastic Sheets

In this talk, we discuss recent work on energy scaling laws for thin elastic sheets subject to a boundary displacement condition consistent with a conical deformation. Under the constraint that the center of the sheet deform only slightly, we derive upper and lower bounds for the elastic energy which agree, up to a factor, with the energy of the associated conical deformation smoothed out near its tip. For a restricted class of boundary deformations, we show that similar energy scaling laws hold without a constraint on the deformation at the sheets center.

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MS57

Pattern Formation in Compressed Elastic Films on Compliant Substrates: An Explanation of the Herringbone Structure

We consider the buckling of a thin elastic film bonded to a thick compliant substrate, when the (compressive) misfit is relatively large. Previous experimental and numerical studies suggest that a herringbone pattern minimizes the total energy (the membrane and bending energy of the film, plus the elastic energy of the substrate). We verify this, by (i) identifying the scaling law achieved by the herringbone pattern, and (ii) proving that no structure can achieve a better scaling law.

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MS57

On the Inability of Continuum Theory to Predict the Elastic Energy of a Strained Alloy Film

An explicit calculation of a ball and spring model shows that while continuum theory can predict the average displacement field for an alloyed system it cannot correctly determine the elastic energy. Implications of this result will be discussed. This is joint work with Christian Ratsch and Arvind Baskaran.

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MS58

Aposteriori Analysis of Multirate and Multiscale Evolution Systems

We consider analysis of numerical methods for multiscale and multirate evolution models that present significantly different temporal and spatial scales within the components of the model. We interpret the multirate method as a multiscale operator decomposition method and use this to conduct both an apriori and a hybrid apriori–aposteriori error analysis. We formulate an iterative multirate Galerkin finite element method then employ adjoint operators and variational analysis. We consider analyses of both ODEs and PDEs.

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MS58

Quantification of Operator Splitting Effects in Finite Volume Calculations of Advection-diffusion

Some issues are presented involving splitting effects near boundaries in operator-split finite volume calculations for advection-diffusion. In applications, it is desirable to understand the errors and sources of errors in calculations, such as splitting effects, which may be difficult to determine. One approach is presented for *a posteriori* error estimation to calculate the error in a quantity of interest (QoI) and investigate the effect of the splitting on the computed QoI value.

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MS58

Consistency and Stability Considerations for Implicit-explicit Additive Splittings

Stability and consistency properties of operator splitting time-marching are challenging to characterize and interpret due to the coupling effects, which lead to complex interactions among operators. In additive splittings the right hand side can be represented as a sum of terms that typically have different properties, such as stiff and nonstiff, and require integrators with different stability properties. We focus on multistage additive implicit-explicit (IMEX) splittings and present new IMEX schemes.

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MS58

Coupling for a Virtual Nuclear Reactor

Abstract not available at time of publication.

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MS59

A Problem of Boundary Controllability for a Plate

The boundary controllability problem, here discussed, might be described by a two-dimensional space equation modeling, at the same time t, different physical phenomena in a composite solid made of different materials. These phenomena may be governed, at the same time t, for example, by the heat equation and Schrödinger equation in two separate regions. Interface transmission conditions are imposed.

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MS59

Mathematical Challenges Arising from the Questions of Controllability for Linked Elastic Structures

A tremendous challenge in the study of control and stabilization of dynamic elastic systems is the ability to rigorously address whether linked dynamic structures can be controlled using boundary feedback alone. When a structure is composed of a number of interconnected elastic elements or is modelled by a system of coupled partial differential equations, the behavior becomes much harder to both predict and to control. This talk focuses on a number of issues that arise when attempting to control these complex systems.

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MS59

Limitations on Control and Stabilization of Certain Hybrid Systems

Hybrid systems are often modeled as continuous parameter systems modeled by partial differential equations coupled to point masses. It is natural to attempt to establish exact controllability and/or uniform exponential stabilizability of the overall system using controls applied to these point masses. We show, using extensions of the notion of the operator trace, that the discrete mass property of such points of control application impose definite limitations on achievement of these goals.

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MS59

Ensemble Dynamics and Bred Vectors

Abstract not available at time of publication.

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MS60

Heated Tear Film in One Dimension with a Moving Boundary

We consider model problems for the tear film over multiple blink cycles with evaporation and with heat transfer from with a model domain for the eye. The nonlinear PDE for film thickness is coupled with heat transfer under the film; simultaneous solution on a moving domain is via a spectral method. The numerical results reveal a similarity to quantitative in vivo observations of the film dynamics and the surface temperature of the film.

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MS60

Fingering Instability of Evaporating Thin Films

The fingering instability of a volatile, viscous liquid flowing down an inclined, heated surface is investigated. A lubrication type approach is used to develop a three-dimensional model of the flow, and numerical simulations are conducted based on the model. Liquids of various wetting properties are considered. Evaporation is found to have a stabilizing influence on the flow, with the strength of evaporation needed to completely suppress the instability increasing with increasing apparent contact angle.

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MS60

A Multiple Scales Approach to Evaporation induced Marangoni Convection

In this talk, we consider the stability of a thin liquid layer of a binary mixture of a volatile (solvent) and a non-volatile (polymer) species. Evaporation depletes the solvent near the liquid surface, which can lead to Bénard-Marangoni-type convection. Due to evaporation, the base state is time dependent, thus impeding the use of normal modes. However, the evaporation is slow on the diffusive time scale, and this is exploited via a systematic multiple scales expansion.

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MS60

Asymptotics of a Thermally Driven Thin Film

A flow driven up an inclined plane by thermal Marangoni stresses is modeled using the lubrication approximation in one dimension, yielding a fourth order nonlinear PDE. Two qualitatively distinct solutions to the steady-state ODE arise when additional localized heating is introduced. Solution type is determined by the magnitude of this localized heating. Solution behavior as a function of this heating parameter is explored using asymptotic analysis and validated through comparison with numerical simulations.

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MS61

Application of Graph Scaffolding in Approximating the Chromatic Number

We introduce the concept of graph scaffolding, through its application in finding the chormatic number of large-scale networks. Graph scaffolding is a a generalized framework for working with combinatorial optimization problems that first exploits theoretical results to compute exact or near-exact solutions on well-defined portions of the graphthe scaffoldand then leverages the answer on the scaffold to construct a high-quality solution to the overall problem. We demonstrate through empirical and theoretical results how by using chordal graphs as a scaffold, the chormatic number of a given graph can be closely approximated.

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MS61

Sparsification Techniques for Metaphor Comprehension

Comprehension of metaphors occurs at the highest level of language proficiency. Metaphor comprehension is computationally challenging as well. The basic technique involves building semantic spaces for words using relevant corpora. Given large scale corpora such as English Wikipedia, sparsification becomes a necessity. In this presentation, we will detail some of the sparsification techniques we have used for metaphor comprehension.

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MS61

Graph Sparsification Methods in Cybersecurity

In cybersecurity and related problem domains we often must deal with very large graphs. For example, consider traffic on a large computer network, a multigraph with upwards of hundreds of thousands of nodes. In order to accomplish tasks like connected component identification, path finding, and subgraph isomorphism in these large network graphs we are turning to graph sparsification. We will describe the sparsification techniques we are using and give an analysis of their performance.

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MS61

Sparse Graph Realization from a Metric Space

We present an approach for constructing a locality graph for set of points in a given metric space, without the need for an underlying geometry on the space. In addition, the graph of all calculated distances is sparse, making our approach appropriate for very high-dimensional data.

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MS62

On Local Refinement via T-splines

We study properties of Analysis Suitable (AS) T-splines which are needed to use T-splines within an adaptive procedure in Isogeometric Analysis. We set up a priori and a posteriori error analysis; we study the use of AS T-splines to solve mixed problems and, more in general, non-coercive differential problems.

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MS62

Challenges in Isogeometric Analysis (IGA)

IGA replaces traditional Finite Elements by watertight structures of 3-variate NURBS. The introduction of NURBS in FEA allows accurate representation of CAD-shapes in FEA. However, efficient technology for establishing watertight IGA-models from CAD-models has to be developed, local refinement of IGA-models has to be improved, and direct GPU-based visualization of IGA-models has to be developed. IGA potentially simplifies analysis of as-is models as the path from measurement through CAD to analysis is shortened.

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MS62

Isogeometric Analysis for Shape Optimization

One of the attractive features of isogeometric analysis is the exact representation of the geometry. The geometry is furthermore given by a relative low number of control points and this makes isogeometric analysis an ideal basis for shape optimisation. I will describe some of the results we have obtained and also some of the problems we have encountered. One of these problems is that the geometry of the shape is given by the boundary alone. And, it is the parametrisation of the boundary which is changed by the optimisation procedure. But isogeometric analysis requires a parametrisation of the whole domain. So in every optimisation cycle we need to extend a parametrisation of the boundary of a domain to the whole domain. It has to be fast in order not to slow the optimisation down but it also has to be robust and give a parametrisation of high quality. These are conflicting requirements so we propose the following approach. During the optimisation a fast linear method is used, but if the parametrisation becomes singular or close to singular then the optimisation is stopped and the parametrisation is improved using a nonlinear method. The optimisation then continues using a linear method.

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MS62

Locally Refined B-splines

We will address local refinement of a tensor product grid specified as a sequence of inserted line segments parallel to the knot lines. We obtain a quadrilateral grid with T-junctions in the parameter domain, and a collection of tensor product B-splines on this mesh here named an LR-mesh. The approach applies equally well in dimensions higher than two. Moreover, in the two dimensional case this collection of B-splines spans the full spline space on the LR-mesh.

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MS63
The Challenges of Robustness in High Dimensions

We consider the problem of dealing with (potentially maliciously) corrupted points in the high dimensional regime. We show that even for basic problems like regression and PCA, existing techniques from robust statistics fail dramatically. We develop new techniques designed for robustness in the high dimensional regime.

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MS63
Compressive Principal Component Pursuit

We consider the problem of recovering target matrix that is a superposition of low-rank and sparse components, from a small set of linear measurements. This problem arises in compressed sensing of videos and hyperspectral images, as well as in the analysis of transformation invariant low-rank matrix recovery. We analyze the performance of the natural convex heuristic for solving this problem, under the assumption that measurements are chosen uniformly at random. We prove that this heuristic exactly recovers low-rank and sparse terms, provided the number of observations exceeds the number of intrinsic degrees of freedom by a polylogarithmic factor. Our analysis introduces several ideas that may be of independent interest for the more general problem of compressed sensing of superpositions of structured signals.

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MS63
Robust Locally Linear Analysis with Applications to Image Denoising and Blind Inpainting

I will talk about the problems of denoising images corrupted by impulsive noise and blind inpainting (i.e., inpainting when the deteriorated region is unknown). Our basic approach is to model the set of patches of pixels in an image as a union of low-dimensional subspaces, corrupted by sparse but perhaps large magnitude noise. For this purpose, we develop a robust and iterative method for single subspace modeling and extend it to an iterative algorithm for modeling multiple subspaces. I will also cover the convergence for the algorithm and demonstrate state of the art performance of our method for both imaging problems.

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MS63
A Novel M-Estimator for Robust PCA

We formulate a convex minimization to robustly recover a subspace from a contaminated data set, partially sampled around it, and propose a fast iterative algorithm to achieve the corresponding minimum. We establish exact recovery by this minimizer, quantify the effect of noise and regularization, explain how to take advantage of a known intrinsic dimension and establish linear convergence of the iterative algorithm. We compare our method with many other algorithms for Robust PCA on synthetic and real data sets and demonstrate state-of-the-art speed and accuracy.

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MS64
Relaxation Results for Nematic Elastomers

We compute the relaxation of a free-energy functional which describes the order-strain interaction in incompressible nematic elastomers in the regime of small strains. Adopting the uniaxial order tensor theory (Frank model) to describe the liquid crystal order, we prove that the minima of the relaxation exhibit an effective biaxial nematic texture (that of the de Gennes theory). The relaxed energy density satisfies a solenoidal quasiconvexification formula. (ARMA 197 N.3, 2010).

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MS64
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS64
A Ginzburg-Landau-type Model for Liquid Crystals

We will discuss some results regarding the Landau-De Gennes energy, often used to model liquid crystals, within the framework developed by Bethuel, Brezis and Helein for the Ginzburg-Landau energy of superconductivity. Our aim is to describe the singularities allowed by this model.

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MS64

Hypertractions and Hyperstresses in Second Gradient Continua

A complete and coherent theory of second gradient continua has not yet been fully developed. Hyperstresses and edge interactions are some of the key features which need to be better understood. We shall review some of the main problems and recent results in this field.

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MS65

Nucleation and Motion of Crystals in a Binary Solution

Abstract not available at time of publication.

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MS65

Pseudo-spectral Simulations of Models for Regularized Dynamic Models in Nonlinear Elasticity

We discuss results of computations of two dimensional viscoelastic models which arise as simplifications of models for phase transformations. These models in include dynamical scalar Aviles-Giga and Kohn-Muller models. We also discuss the resulting nature of energy minimizing solutions that are obtained from numerical simulations of these models. Finally, we show that some similar results can be obtained in vectorial two dimensional models for martensitic phase transformations.

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MS65

Wrinkling of a Floating Elastic Film: Energy and Pattern

In this talk, I discuss the floating film problem in which a rectangle elastic film floats on the surface of a pool of liquid and is compressed along two opposing sides. I first present the energy scaling law and then show how to use it to explain the cascade pattern at the edges of the two other sides of the film observed experimentally.

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MS65

Conical Singularities in Thin Elastic Sheets

When one slightly pushes a thin elastic sheet into a hollow cylinder, the resulting configuration of the sheet is a so-called d-cone. D-cones have drawn some attention in the physics community in the last two decades or so, see e.g. Cerda et al., Nature 401, 46 (1999). In this talk, we examine the scaling of the elastic energy with the sheet thickness h in a rigorous setting and give a lower bound that is optimal in the leading order of h.

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MS66

Searching for Exceptional Mechanisms with Fiber Products

Given a family of mechanisms and its parameterized system of equations, techniques from Numerical Algebraic Geometry can be used to find mechanisms with greater than expected motion. The parameters of such mechanisms can be found using the fiber product technique of Sommese and Wampler to uncover irreducible sets that are obscured within a larger algebraic set. Applications to particular families of mechanisms and adaptations for dealing with large sets of defining equations will be discussed.

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MS66

Quasi Steady State Solution and Bifurcation for a Cell Cycle Model

We consider a free boundary problem for a system of partial differential equations, which arises in a model of tissue growth. For the steady state system, it depends on a positive parameter β, which describes the signals from the microenvironment. Upon discretizing this model, we obtain a family of polynomial systems parameterized by β. We numerically find that there exists a radially-symmetric stationary solution with tumor free boundary $r = R$ for any given positive number R. By homotopy tracking with respect to the parameter β, there exist branches of symmetry-breaking stationary solutions. Moreover, we proposed a numerical algorithm based on Crandall-Rabinowitz theorem to numerically verify the bifurcation points. By continuously changing μ using a homotopy, we are able to compute nonradial symmetric solutions. We additionally discuss optimal control on β.

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MS66

Real Solutions to Polynomial Systems Arising in Mechanism Design

Parameterized polynomial systems naturally arise in many applications, including mechanism design. This talk will explore using techniques from numerical algebraic geometry to attempt to compute parameters for which the polynomial system has an extremal number of real solutions. An example from mechanism design will be used to demonstrate the approach where there exists a set of parameters for which the corresponding system has no real solutions and a set of parameters for which the corresponding system has all solutions real.

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MS66

Cell Decomposition of Real Surfaces Defined by Mechanism Motions

This talk will describe the application of numerical algebraic geometry to decompose a real algebraic surface into a cell structure. A general technique for almost smooth algebraic surfaces will be reviewed and then applied to several mechanisms. An interesting case is the study of one-degree-of-freedom mechanisms with one free design parameter, such as a link length. The cell decomposition finds critical values of the parameter where the topology of the motion curve changes.

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MS67

Multilevel Algorithms for Stokes Type Systems

We analyze multilevel algorithms for symmetric saddle point systems. We combine inexact Uzawa algorithms at the continuous level with Uzawa and gradient type algorithms at the discrete level. The algorithms are based on the existence of multilevel sequences of nested approximation spaces that do not have to satisfy a discrete LBB stability condition. The main idea is to maintain an accurate representation of the residuals at each step of the inexact Uzawa algorithm at the continuous level. The residual representations at each step are approximated by projections. Iteration on a fixed level corresponds to standard Uzawa or Gradient method for solving symmetric saddle point systems. Whenever a sufficient condition for the accuracy of the representation for the main residual (of the first equation) fails to be satisfied, the representation is projected on the next larger space. We emphasize on the gradient method which has the advantages of automatically selecting the relaxation parameter, lowering the number of iterations on each level, and improving on running time and on global error reduction. Numerical results are presented for the Stokes system.

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MS67

HDG Methods for the Vorticity-Velocity-Pressure Formulation of the Stokes Problem

In this talk we discuss the hybridizable discontinuous Galerkin (HDG) method for solving the vorticity-velocity-pressure formulation of the three-dimensional Stokes equations of incompressible fluid flow. The idea of the *a priori* error analysis consists in estimating a projection of the errors that is tailored to the very structure of the numerical traces of the method. We show that the approximated vorticity and pressure, which are polynomials of degree k, converge with order $k + 1/2$ in L^2-norm for any $k \geq 0$. Moreover, the approximated velocity converges with order $k + 1$.

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MS67

An Alternative Multigrid Method for Incompressible Flow

A multigrid method for H(div)-conforming DG discretizations of the Stokes problem is presented. It is based on an overlapping domain decomposition smoother. The smoother operates in thedivergence free subspace and thus does not require to be embedded into a block preconditioner for the saddle point problem. It is proven that the method is a uniform preconditioner.Its efficiency is documented with numerical examples.

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MS67

Flow in Pebble Bed Geometries

Flow in complex geometries intermediate between free flows and porous media flows occurs in pebble bed reactors and in optimization of turbine placement in wind farms. The Brinkman models have consistently shown that for simplified settings accurate prediction of essential flow features depends on the impossible problem of meshing the pores. In this paper we investigate new model to understand the flow and its properties in these geometries.

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MS68

The Importance of the Inner-problem in Computational Models of Dynamic Brittle Fracture and why Peridynamics Works

I discuss the importance of capturing the "inner-problem' in modeling dynamic fracture. The mechanism for crack branching proposed by experimentalists suggests that when the S.I.F. becomes sufficiently high, voids grow into microcracks ahead of the crack tip. I argue that computational models which are not able to represent the evolution of these microcracks, will not be able to correctly predict dynamic brittle fracture. Peridynamics, a nonlocal extension of classical mechanics, accounts implicitly for microcracks by the way in which nonlocal damage evolves in this theory.

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MS68

Peridynamic Energy Balance and Damage

Our presentation reviews the recently proposed nonlocal energy balance for peridynamic solids. Appropriate expressions for the first and second laws of thermodynamics are given, including a justification using the principles of non-equilibrium statistical mechanics. The first law expression explicitly includes nonlocal interactions in a term that represents the stress power in peridynamic theory. The second law enables restrictions to be placed on constitutive relations and is demonstrated to be a generalization of the Coleman-Noll procedure. An application to damage is presented.

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MS68

The Peridynamic J-integral

In fracture mechanics, the J-integral characterizes the energy balance for a growing crack. In the nonlocal peridynamic version of the J-integral, the rate of work done on the contour is replaced by a volume integral of work done on the bonds that connect the inside to the outside of the contour. The peridynamic J-integral converges to the standard version in the limit of small horizon. Numerical examples compare values in the peridynamic and standard theories.

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MS68

The Effect of Surface Tension on the Stress Field near a Curvilinear Crack

In this talk, an approach to modeling fracture incorporating interfacial mechanics is applied to the example of a curvilinear plane strain crack. The classical Neumann boundary condition is augmented with curvature-dependent surface tension. It is shown that the considered model eliminates the integrable crack-tip stress and strain singularities of order 1/2 present in the classical linear fracture mechanics solutions, and also leads to the sharp crack opening that is consistent with empirical observations.

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MS70

Cocircuits of Linear Matroids

We present a set covering problem (SCP) formulation of the matroid cogirth problem. Addressing the matroid cogirth problem can lead to significantly enhancing the design process of sensor networks. The solution to the matroid cogirth problem provides the degree of redundancy of the corresponding sensor network, and allows for the evaluation of the quality of the network. We provide computational results to validate a branch-and-cut algorithm that addresses the SCP formulation.

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MS70

Recent Advances in Optimization Methods for Image Processing

Nonlinear image reconstruction based upon sparse representations of images has received widespread attention recently with the advent of compressed sensing. This emerging theory indicates that, when feasible, judicious selection of the type of distortion induced by measurement systems may dramatically improve our ability to perform reconstruction. In this talk, we discuss some recent advances in large-scale optimization methods for solving these sparse signal recovery problems.

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MS70

Approximate Murphy-Golub-Wathen Preconditioning for KKT Matrices

Karush-Kuhn-Tucker matrices arise from first order necessary conditions for nonlinear optimization. Murphy, Golub, and Wathen proposed a preconditioner having three distinct eigenvalues, giving exact GMRES convergence in three iterations. This ideal preconditioner involves the inverse of a large submatrix, but when computed inexactly, GMRES will no longer converge in three steps. How will this compromise slow convergence? Recent results on the stability of GMRES give rigorous bounds on the number of iterations. Numerical computations verify these results for problems from optimization and fluid dynamics.

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MS70

Recent Results on the Smallest Enclosing Ball Problem and the Smallest Intersecting Ball Problem

In the 19th century, J.J. Sylvester introduced the smallest enclosing circle problem: find a circle of smallest radius enclosing a given set of finite points on the plane. We extend the problem and find a ball with the smallest radius that encloses a finite number of nonempty closed sets. Similarly, we study the smallest intersecting ball problem. Necessary and sufficient optimality conditions will be presented, as well, as numerical results. Applications exist in the field of facility location.

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MS71

Markovian Projection of Stochastic Processes

We give conditions under which the flow of marginal distributions of a discontinuous semimartingale can be matched by a Markov process whose infinitesimal generator can be expressed in terms of its local characteristics, generalizing a result of Gyongy (1986) to the discontinuous case. Our construction preserves the martingale property and allows to derive a partial integro-differential equation for the one-dimensional distribution of discontinuous semimartingales, extending the Kolmogorov forward equation (Fokker Planck equation) to a non-Markovian setting.

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MS71

Functional Ito Calculus and PDEs on Function Spaces

The Functional Ito Calculus (Dupire 2009 ; Cont & Fournie 2010) is a calculus for non-anticipative functionals on the space of right-continuous paths, which extends the Ito calculus to path-dependent functionals of stochastic processes (Cont & Fournie 2011). This calculus, applied to functionals of a martingale, leads to a new class of PDEs on the space of continuous functions, which share various properties with parabolic PDEs in finite dimensions : comparison principle, maximum principle, functional Feynman-Kac formula. In particular, we characterize Brownian martingales as weak solutions of a functional heat equation.

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MS71

Viscosity Solutions of Path Dependent PDEs

We propose a notion of viscosity solutions for path dependent parabolic PDEs. This can also be viewed as viscosity solutions of non-Markovian control problems, and thus extends the well known nonlinear Feynman-Kac formula to non-Markovian case. We shall prove the existence, uniqueness, stability, and comparison principle for the viscosity solutions. The key ingredient of our approach is a functional Itos calculus recently introduced by Dupire and further developed by Cont-Fournie.

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MS71

Control of Non-Markovian Stochastic Differential Equations

We study stochastic differential equations (SDEs) whose drift and diffusion coefficients are path-dependent and controlled. We construct a value process on the canonical path space, considered simultaneously under a family of singular measures, rather than the usual family of processes indexed by the controls. This value process is characterized by a second order backward SDE, which can be seen as a non-Markovian analogue of the Hamilton-Jacobi-Bellman partial differential equation.

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MS72

Adaptive Split-operator Methods for Modeling Flow and Transport Phenomena in Porous Medium Systems

Split-operator methods facilitate computation of large coupled problems. However, these methods introduce splitting error, which is typically either ignored or controlled heuristically. In this work, we develop algorithms to control the splitting error by dynamically adapting the temporal splitting step based upon error estimators. The methods yield robust and efficient solutions with error control for nonlinear reaction problems and can be extended to Navier-Stokes and multiphase problems. These algorithms have widespread applicability in environmental modeling.

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MS72

An IMEX Method for the Euler Equations That Posses Strong Non-Linear Heat Conduction and Stiff Source Terms (Radiation Hydrodynamics)

We present a truly second order time accurate self-consistent IMEX (IMplicit/EXplicit) method for solving the Euler equations that posses strong nonlinear heat conduction and very stiff source terms (Radiation hydrodynamics). IMEX methodology is suggested when dealing with physical systems that consist of multiple physics or fluid dynamics problems that exhibit multiple time scales such as advection-diffusion, reaction-diffusion, or advection-diffusion-reaction. It can be challenging to provide fully converged and second order time accurate numerical results to these kinds of coupled systems. Order reductions in time accuracy are often reported due to inconsistent operators splitting. Our JFNK (Jacobian-Free Newton Krylov)-based IMEX method splits the operators in a self-consistent way in which all-non-linearities are converged and second order time accuracy of different physical terms is preserved. We have applied this strategy to a Radiation Hydrodynamics model (at diffusion approximation limit) that posses multi-scale terms and demonstrated second order time accuracy.

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MS72

Operator Splitting Integration Factor Methods for Complex Biological Systems

For reaction-diffusion-advection equations, the stiffness from the reaction and diffusion terms often requires very restricted time step size, while the nonlinear advection term may lead to a sharp gradient in localized spatial regions. It is challenging to design numerical methods that can efficiently handle both difficulties. For reactiondiffusion systems with both stiff reaction and diffusion terms, implicit integration factor (IIF) method and its higher dimensional analog compact IIF (cIIF) serve as an efficient class of time-stepping methods, and their second order version is linearly unconditionally stable. Here we use splitting methods to incorporate different numerical methods to handle different terms of the equations. In particular, we apply the IIF-cIIF method to the stiff reaction and diffusion terms and the WENO method to the advection term in two different splitting sequences. Calculation of local truncation error and direct numerical simulations for both splitting approaches show the second order accuracy of the splitting method, and linear stability analysis and direct comparison with other approaches reveals excellent efficiency and stability properties. Applications of the splitting approach to several biological systems demonstrate that the overall method is accurate and efficient.

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MS72

Reduced Description of Reactive Flows with Tabulation of Chemistry

Reduced description with chemistry tabulation can effectively reduce the simulation time of reactive flows by solving the evolution equations only for represented species. With operator splitting, chemical reactions are separated into a reaction fractional step. The effect of chemical reactions on the reduced composition is addressed through species reconstruction and the evaluation of reaction mapping in the full composition space. ISAT is employed to speed chemistry calculation by tabulating information of the reduced system.

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MS73

Multiscale Engineering for Heterogeneous Media and Structures

In this talk, we present multiscale materials design success stories and discuss some technical barriers to using multiscale simulation for rapid materials design and qualification. A paradigm for computational multiscale modeling and simulation will be discussed which, when integrated into the structural design loop, will significantly expand the design space and enable increased efficiency, performance, and affordability by delivering materials and structures optimized across all engineered scales for their mission.

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MS73

Development of Computational Algorithms for Materials Simulation and Design

Supported first by NSF-ITR then by the NSF-IUCRC center for computational materials design, we have worked on a number of mathematical and algorithmic issues that are related to efficient and multiscale simulation of various physical processes such as nucleation and coarsening during phase transformations. In this talk, we will discuss some of our recent works, including the development of algorithms for predicting critical nuclei morphology in anisotropic elastic solids, the study of coarsening kinetics of a mixture with disparate mobility and the uncertainty quantification and statistical assessment of database used for material property optimization.

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MS73

The Role of SIAM As An Advocate for the Mathematical Science Community

This presentation will describe the efforts of SIAM to advocate for the interests of the mathematical sciences community with policy makers and funding agencies, including the activities of the SIAM Committee for Science Policy. The presentation will also detail ways in which the SIAM membership can participate in this effort.

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MS73

Materials Genome: An Opportunity for Applied Mathematics and Computational Science

The recent Materials Genome Initiative seeks to accelerate the process between materials discovery and their industrial application. In this talk we highlight problems where computational science and mathematics can play a role in materials innovation and development.

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MS74

Staggered Discontinuous Galerkin Method for Wave Transmission Between Dielectric and Metamaterials

Some electromagnetic materials exhibit, in a given frequency range, effective dielectric permittivity and/or magnetic permeability which are negative. In the literature, they are called negative index materials, left-handed materials or meta-materials. We propose a staggered discontinuous Galerkin method to solve a wave transmission between a classical dielectric material and a meta-material. Convergence of the numerical method is proven, with the help of explicit inf-sup operators, and numerical examples are provided to show the efficiency of the method.

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MS74

HDG Methods for Wave Propogation

We describe the devising and analysis of the so-called hybridizable discontinuous Galerkin method for the acoustic equation in the time-continuous domain. The method provides optimal approximations for the velocity, the gradient and the original scalar unknown. A superconvergence property of the velocity allows us to obtain a new approximation to the original scalar unknown converging with one additional order.

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MS74

Eulerian Gaussian-beams in the Viscosity Sense for Multidimensional Schrodinger Equation in the Semi-classical Regime

We design an Eulerian Gaussian-beam method for the Schrodinger equation in the semi-classical regime, where the Planck constant is small. The method is constructed from a leading-order WKBJ ansatz for the quantum wave function, where the phase and the amplitude satisfy an eikonal and a transport equation respectively. The transport equation is weakly coupled to the eikonal equation in the sense that one must first solve the eikonal equation to provide related coefficients for the transport equation. We use a high-order numerical scheme to evolve the set of equations to get a highly efficient and accurate approximation of the Schrodinger equation in multidimensions.

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MS74
Is a Curved Flight Path in SAR Better than a Straight One?

We study the simplified model of Synthetic Aperture Radar imaging: recovery of singularities of a function in the plane by knowing integrals along circles centered at a given curve (the flight path). If the curve is a straight line, the symmetry about it cannot be resolved. It has been suggested that a curved flight path might be better to break the symmetry. We show that in some sense (local measurements), a curved path is not better but a closed (and of course, curved) path offers some advantages. Our approach is based on wave propagation methods and provides constructive algorithms for reconstruction in some cases. This is a joint work with Gunther Uhlmann.

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MS75
Investigating through Optimal Control of Parabolic PDEs: Does Movement Toward a Better Resource Benefit a Population?

We investigate optimal control of the convective coefficient in parabolic parabolic partial differential equation, modeling a population with nonlinear growth. This work is motivated by the question: Does movement toward a better resource environment benefit a population? Results on existence, uniqueness, and characterization of the optimal control will be presented along with numerical illustrations. This work is in collaboration with Tuoc Phan and Heather Finotti.

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MS75
Stabilization of Wave Equations with Wentzell Boundary Conditions

I will discuss uniform feedback stabilization of wave equations subject to second-order boundary conditions. Both dynamic (Wentzell) and static (higher derivatives in space only) boundary conditions will be considered. It will be shown how a combination of a partially localized boundary feedback and a partially localized collar feedback leads to uniform energy decay rates. The analysis combines weighted energy methods for observability of Neumann-type wave problems and differential-geometric techniques for proving stability of waves on compact manifolds.

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MS75
Asymptotic Behavior in a 2-allele Genetic Model with Population Control

The standard model for the evolution of the densities of the three genotypes aa, aA, and AA is $\partial\rho_{aa}/\partial t - \Delta\rho_{aa} = r[2\rho_{aa} + \rho_{aA}]^2/\{2[\rho_{aa} + \rho_{aA} + \rho_{AA}]\} - \tau_{aa}\rho_{aa}$ $\partial\rho_{aA}/\partial t - \Delta\rho_{aA} = 2r[2\rho_{aa}+\rho_{aA}][2\rho_{AA}+\rho_{aA}]/\{2[\rho_{aa}+\rho_{aA}+\rho_{AA}]\} - \tau_{aa}\rho_{aa}$ $\partial\rho_{AA}/\partial t - \Delta\rho_{AA} = r[2\rho_{AA} + \rho_{aA}]^2/\{2[\rho_{aa} + \rho_{aA} + \rho_{AA}]\} - \tau_{AA}\rho_{aa}$,
where the parameters are constants. It has recently been shown by Souplet and Winkler that in the heterozygote intermediate case $\tau_{aa} \geq \tau_{aA} \geq \tau_{AA}$, $\tau_{aa} > \tau_{AA}$ the gene fraction $u := [2\rho_{aa} + \rho_{aA}]/\{2[\rho_{aa} + \rho_{aA} + \rho_{AA}]\}$ converges to 0. However, the proof in the biologically interesting case depends on the fact that ρ_{AA} converges to infinity, which, as the authors pointed out, makes the model unrealistic. We produce a large class models of the above form with the birth rate r replaced by a density-dependent function and no terms dropped which have the property that when the population lives in a bounded domain with impenetrable boundary and its initial conditions satisfy some reasonable conditions, then as the time approaches infinity, the population densities converge uniformly to those of a constant equilibrium in which the allele a is absent.

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MS75
Quasi-Stationary Limit and Landau-Lifshitz Equations Without Exchange Energy

In this paper we study a dynamic model of Landau-Lifshitz equations in ferromagnetism that do not include exchange energy. The weak solution to such an equation is obtained as the quasi-stationary limit of a simple coupled Maxwell system when dielectric permittivity approaches zero. We present a new direct proof of this quasi-stationary limit result and also establish a finite-time local L^2-stability result and thus the uniqueness for the weak solutions with bounded initial data.

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MS76
Quadratic Sum of Squares Relaxations

We consider the question of minimizing a quadratic objective function over a real variety described by quadratic equations. This problem is NP-hard in general. We give necessary and sufficient conditions in terms of Lagrange multipliers under which the first sum of squares relaxation is exact, assuming attainment of both the SOS relaxation and the original objective. We apply the theorem when the objective is squared Euclidean distance to a point, where we see that these methods can effectively tackle image reconstruction problems in computer vision which motivated this work.

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MS76

Positive Gorenstein Ideals

I will explain how positive Gorenstein ideals arise naturally from the dual cone to the cone of sums of squares. The structure of these ideals provides a new tool for addressing questions of nonnegative polynomials and sums of squares. I will present applications in algebraic geometry, analysis and optimization. In particular there is a simple proof of Hilbert's result on representation of ternary forms as sums of squares of rational functions.

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MS76

Algebraic Structure in Optimization

Solving polynomial optimization problems is known to be a hard task in general. In order to turn the recently emerged relaxation paradigms into efficient tools for these optimization questions it is necessary to exploit further structure whenever presented in the problem structure. In this talk we will focus on the situation of optimization problems that are given by symmetric polynomials in order to highlight several approaches to take advantage of symmetry. The techniques presented in the talk will also give a better understanding of the cones of symmetric sums of squares and symmetric non negative forms and the symmetric mean inequalities associated to these. In particular, we will show that in degree four, symmetric mean inequalities are characterized by sum of squares decomposition.

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MS76

Regularization Methods for SDP Relaxations in Large Scale Polynomial Optimization

In this talk, we discuss how to solve semidefinite programming relaxations for large scale polynomial optimization. When interior-point methods are used, only small or moderately large problems could be solved. Here we use regularization methods on semidefinite programming with block structures, and significant bigger problems could be solved on a regular computer, which is almost impossible by interior point methods. The performance is tested on various numerical examples. Some numerical issues are also discussed.

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MS77

A Continuous Multilevel Solver for the Vertex Separator Problem

Given an undirected graph G, the vertex separator problem is to find the smallest number of nodes whose removal disconnects the graph into disjoint subsets A and B, where A and B are subject to size constraints. We will show how this problem can be formulated as a continuous quadratic program. We use the QP as a local processor in a multilevel scheme for solving large scale instances of the problem. Computational results will be presented.

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MS77

An Exact Algorithm for Graph Partitioning based on Quadratic Programming

Abstract not available at time of publication.

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MS77

Exact Combinatorial Branch-and-bound for Graph Bisection

We present a novel exact algorithm for the minimum graph bisection problem, whose goal is to partition a graph into two equally-sized cells while minimizing the number of edges between them. Our algorithm is based on the branch-and-bound framework and, unlike most previous approaches, it is fully combinatorial. We present stronger lower bounds, improved branching rules, and a new decomposition technique that contracts entire regions of the graph without losing optimality guarantees. In practice, our algorithm works particularly well on instances with relatively small minimum bisections, solving large real-world graphs (with tens of thousands to millions of vertices) to optimality.

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MS77

Multi-Level Edge Separator Using a Hybrid Combinatorial-Quadratic Programming Approach

The graph partitioning problem arises in a variety of scientific and engineering domains such as VLSI design, computer networking, parallel computing, and sparse direct methods. In this talk, we discuss the edge separator graph partitioning problem and present an algorithm which combines aspects of multi-level combinatorial methods with a quadratic programming formulation. We discuss a novel strategies for both graph coarsening and refinement with the goal of producing high quality cut sets.

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MS78
The Geometry of Interpolation Error Estimates for Isogeometric Analysis

Barycentric coordinates provide a basis for linear finite elements, and underlie the definition of higher-order basis functions for shape and isogeometric analysis, i.e. the Bézier triangle in computer aided-design, together with interpolation and shading techniques in computer graphics and optimal convergence rates in isogeometric analysis. The versatility of this construction has led to barycentric coordinates for more general shapes; the resulting functions are called generalized barycentric coordinates (GBCs). GBCs while unique over triangles, have multiple definitions for convex polygons with four or more sides, namely Harmonic (H), Wachspress(W), Sibson (S) and Mean Value (MV) coordinates. Interpolation properties of H, W, S and MV have a complex dependence on polygonal geometry. W exhibits the subtleties of geometrical dependence: if the polygon contains interior angles near 180 degrees, gradients of the coordinates become very large. S and MV avoid this problem. In this talk we prove that given certain conditions on the geometry of the polygon, each of H, W, S and MV can obtain optimal interpolation convergence estimates, and hence suitable for isogeometric analysis.

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MS78
Analysis Aware Representations, Parameterizations, and Models

Isogeometric Analysis (IA) has been proposed as a methodology for bridging the gap between Computer Aided Design (CAD) and Finite Element Analysis (FEA). In order to support design and full 3D IA, new ab initio design methods must create suitable representations and approximation techniques must include parameterization methodologies for volumes. This presentation discusses some of the challenges in moving from current representations and datafitting techniques towards this goal and demonstrates initial results and analyses.

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MS78
Applications of Isogeometric Analysis at Boeing

Isogeometric analysis at Boeing has a surprisingly long history. Univariate applications using B-splines as finite elements have existed since the late 1980s, with numerous applications. The essence of isogeometric analysis – using a fixed parameter space to formulate a family of problems – was employed in an aeroelastic tool in the late 1990s. That application entailed solving boundary integral equations for a family of surfaces, requiring a form of bivariate isogeometric analysis. We will explore those and future Boeing applications of this exciting technology.

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MS78
Solid T-spline Construction from Boundary Representations

We present a novel method to construct solid rational T-splines for complex genus-zero geometry from boundaries. We first build a parametric mapping between the triangulation and a unit cube. After that we adaptively subdivide the cube using an octree subdivision, pillow the subdivision result one layer on the boundary, and use templates to handle extraordinary nodes. The obtained solid T-spline is C2-continuous except for the local region around each extraordinary node.

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MS79
Posterior Rates of Contraction for Sparse Bayesian Models

Sparse inverse covariance matrix modeling is an important tool for learning relationships among different variables in a Gaussian graph. Most existing algorithms are based on ℓ_1 regularization, with the regularization parameters tuned via cross-validation. In this talk, a Bayesian formulation of the problem is proposed, where the regularization parameters are inferred adaptively and cross-validation is avoided. Variational Bayes (VB) is used for the model inference. Results on simulated and real datasets validate the proposed approach. In addition, a graph extension algorithm is proposed to include a new variable in an existing graph, which can be used when separate testing data are available.

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MS79

Clustering and Embedding of High-Dimensional Multi-Manifold Data using Sparse Representation

In many problems across different areas of science and engineering, we are dealing with massive collections of high-dimensional data. Having thousands and millions of dimensions, the data often lie in or close to low-dimensional structures, called manifolds. Separating the data into the underlying low-dimensional models and finding compact representations for them is one of the most fundamental problems in the high-dimensional data analysis. We address the problem of clustering and embedding of the data on multiple manifolds using sparse representation techniques. We use the collection of the data points as a self-expressive dictionary in which each point can be efficiently represented as a sparse combination of a few other points from the same manifold with appropriate weights that encode locality information. We propose a convex optimization program whose solution is used in a spectral graph theory framework to infer the clustering and embedding of the data. When the manifolds correspond to low-dimensional subspaces, we show that under appropriate conditions on the principal angles between the subspaces and the distribution of the data, the solution of the proposed convex program recovers the desired solution. We demonstrate the effectiveness of the proposed algorithm through experiments on several real-world problems.

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MS79

Poisson Tensor Factorization for Sparse Count Data

In data mining and analysis, we often encounter data that is indexed by three or more indices. Tensor factorizations can be used for such ”multidimensional” data and have already found application in a variety of fields, including high-dimensional function approximations, signal processing, chemometrics, multi-attribute graph analysis, image recognition, and more. We consider the problem of tensor factorizations for sparse count data. For example, we might have a collection of email messages and arrange them by sender, receiver, and date; the data is sparse because not all potential senders and receivers communicate and even those that do communicate do not necessarily do so every day. Typically, we would fit a tensor factorization model to data by minimizing the least squares difference between the data and the tensor factorization model. Statistically speaking, we have assumed that the random variation is best described by a Gaussian distribution. We propose, however, that the random variation may be better described via a Poisson distribution because the count observations (especially the zeros) are more naturally explained. Under this Poisson assumption, we can fit a model to observed data using the negative log-likelihood score, also known as Kullback-Leibler divergence. We discuss an alternating optimization approach and propose solving the subproblem using a majorization-minimization approach that yields multiplicative updates. In fact, the method we propose is a generalization of the Lee-Seung multiplicative updates but has the advantage of being faster and also having provable convergence even for solutions on the boundary (i.e., with zeros in the factorization). Moreover, we show how to prevent the algorithm from converging to non-stationary points (i.e., fixing the problem of getting stuck at undesirable zero values). We will show several examples to demonstrate the utility of the approach.

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MS79

Performance Limits of Non-local Means

In this talk I describe a novel theoretical characterization of the performance of non-local means (NLM) for noise removal. NLM has proven effective in a variety of empirical studies, but little is understood fundamentally about how it performs relative to classical methods based on wavelets or how various parameters (e.g., patch size) should be chosen. For cartoon images and images which may contain thin features and regular textures, the error decay rates of NLM are derived and compared with those of linear filtering, oracle estimators, variable-bandwidth kernel methods, Yaroslavskys filter and wavelet thresholding estimators. The trade-off between global and local search for matching patches is examined, and the bias reduction associated with the local polynomial regression version of NLM is analyzed. The theoretical results are validated via simulations for 2D images corrupted by additive white Gaussian noise. This is joint work with Ery Arias-Castro and Joseph Salmon.

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MS80

Local Pointwise a posteriori Gradient Error Bounds for the Stokes Equations

We consider the standard Taylor-Hood finite element method for the stationary Stokes system on polyhedral domains. We prove local a posteriori error estimates for the maximum error in the gradient of the velocity field. Because the gradient of the velocity field blows up near re-entrant corners and edges, such local error control is necessary when pointwise control of the gradient error is desirable. Computational examples confirm the utility of our estimates in adaptive codes.

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MS80

Mixed Finite Elements for the Coupling of Fluid Flow with Porous Media Flow

In this talk we a introduce mixed finite element method for the coupling of fluid flow with porous media flow. Flows are governed by the Stokes and Darcy equations, respectively, and the corresponding transmission conditions are given by mass conservation, balance of normal forces, and the Beavers-Joseph-Saffman law. We consider mixed formulations in both the Stokes domain and the Darcy region, which yields the introduction of the traces of the porous media pressure and the fluid velocity as suitable Lagrange multipliers. Then, considering generic finite element spaces with some technical conditions, we apply the Babuška-Brezzi theory together with a classical result on projection methods for Fredholm operators of index zero to show stability, convergence, and a priori error estimates for the associated Galerkin scheme. Finally, we generalize the previous results and introduce a mixed finite element method for the coupling of fluid flow with nonlinear porous media flow.

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MS80

A Space-Time Hybridizable Discontinuous Galerkin (HDG) Method for Incompressible Flows on Deforming Domains

We present the first space-time HDG finite element method for the incompressible Navier-Stokes and Oseen equations. Major advantages of a space-time formulation are its excellent capabilities of dealing with moving and deforming domains and grids and its ability to achieve higher-order accurate approximations in both time and space by simply increasing the order of polynomial approximation in the space-time elements.

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MS81

Math modeling as the core of Applied Math undergraduate Curricula

Abstract not available at time of publication.

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MS82

Manycore-portable Multidimensional Arrays for Finite Element Computations

Performance-portability to multicore-CPU and manycore-accelerator (e.g., GPGPU) devices is a significant challenge due to device-specific programming models and performance characteristics. The Kokkos multidimensional array library uses C++ template meta-programming to provide performance-portable multidimensional array data structures and data parallel algorithm dispatch capabilities (e.g., parallel-for and parallel-reduce). These data structures and dispatch capabilities are demonstrated by compiling and executing the same finite element mini-application codes on NUMA multicore-CPU (Intel and AMD) and GPGPU manycore-accelerator (NVIDIA) devices.

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MS82

Asynchronous, Performance-portable Krylov Methods on Accelerators

In this presentation we discuss our efforts to use the Trilinos/Kokkos multi-dimensional array package to write portable generic code implementing the GMRES iterative method. Performance results from several distinct platforms are presented.

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MS82

Auto-Tuned Hybrid Asynchronous Krylov Iterative Eigensolvers on Petascale Supercomputers

Asynchronous hybrid parallel Krylov co-methods, such as the Multiple Explicitly Restart Arnoldi Method (MERAM), are well adapted for Petascale supercomputing. Each ERAM may exploit all parallelism of a large number of processors and asynchronously exchange Ritz elements with the other concurrent methods. Each ERAM may have a dedicated restart strategy to accelerate the convergence to different eigensubspaces. We study the orchestration of different strategies with respect to several distributions along the ERAM methods. We propose to overview these strategies and to evaluate experimentally their efficiencies on a Petascale computer. As a conclusion, we propose an algorithm to auto-tune these strategies and we discuss the first results.

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MS82

Retrofitting a Production Sparse Linear Algebra Library for Accelerators

The Trilinos Epetra package provides most of the current production quality matrix and vector services for other Trilinos packages. Although new packages have emerged (Tpetra and Kokkos) to fundamentally address the next generation of computing needs, especially support for emerging architectures, there is merit in providing some support for new architectures in Epetra. In this talk we discuss efforts to retrofit Epetra with support for accelerators, highlighting design constraints and benefits of the effort.

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MS83

Spatio-temporal Dynamics of 2009 A/H1N1 Influenza

We provide a quantitative description of the age-specific and regional 2009 A/H1N1 pandemic incidence patterns in Mexico and Peru. We analyze the geographic spread of the pandemic waves and their association with the winter school closing periods, demographic factors, and absolute humidity. Our results indicate substantial regional variation in pandemic pattern and highlight the importance of school cycles on the transmission dynamics of pandemic influenza.

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MS83

Game Theory and Vaccination with a Network Epidemiology Approach

Abstract not available at time of publication.

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MS83

The Implications of Different Probability Density Functions for Disease Stages from Sir Epidemiological Models on the Effectiveness of Public Health Interventions

Quantifying the uncertainty attributed to the assumed probability density functions for disease stages from SIR epidemiological models is crucial. Hence, the lack of it might leads to i) limited statements with respect to the net effectiveness of intervention strategies or ii) proposing the implementation of inadequate or non-optimal intervention strategies and thus, these might increase the risks of high mortality and morbidity and misguide public health policy and decision makers. We illustrated that these assumptions quantitatively matter greatly.

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MS83

Modeling the Effect of Hospital Acquired Infections in the Outcomes of Neurosurgical Patients

Abstract not available at time of publication.

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MS84

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS84

Atomic Properties Database Development and Mining for Materials Genome Applications

Exploiting correlations between materials macroscopic properties and atomic properties of their constituents is at the heart of materials informatics whose main goal is to significantly reduce the time to unravel materials with desirable properties. We have initiated a series of studies to explore such correlations by using data mining techniques. This talk will summarize these studies and address specifically the questions: How to build the needed databases and how to use them effectively?

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MS84
Renewable Polymers for a Sustainable Future

Polymers are essential to myriad technologies we encounter every day. Over the past century an immense and highly integrated knowledge base has evolved that guides the manipulation of petroleum feedstocks, the design of polymerization catalysts, and the resulting structure - property relationships in a small set of relatively simple homopolymers. Yet the production and disposal of these products presents inescapable environmental challenges that are costly to correct at a minimum and unsustainable in the long term. In response to a global mandate for sustainability, the development of alternatives based on renewable feedstocks such as carbohydrates, plant oils, and terpenes is of central importance. Realizing the tremendous market potential for bio-based materials hinges on creating new fundamental chemistry-based foundations upon which an industry can be established. Many known sustainable homopolymers have inadequate property profiles to meet the application requirements of modern polymeric materials. Researchers in the Center for Sustainable Polymers (CSP) at the University of Minnesota (UMN) are establishing a comprehensive knowledge base that enables the efficient and economical conversion of natural and abundant molecules into tomorrows advanced polymeric materials. Members of the CSP blend efforts in polymer design, monomer synthesis, polymerization catalysis, architecture and morphology control, and polymer property optimization to establish the basic scientific tenants for innovative renewable resource polymer technologies. A key and unifying concept in the CSP is that multiple renewable components, properly integrated into a single material, will yield tunable properties not achievable with either simple homopolymers or blends, which have dominated the renewable polymer industry to date.

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MS84
Mesoscale Description of Defected Materials

A mesoscale description is necessary for a quantitative description of defected materials, including microstructure evolution. Not only they naturally incorporate defect solutions, but they also permit numerical computation on the diffusive time scales that are appropriate for overdamped defect motion. We describe the general methods involved in the derivation and validation of such models, and apply them to grain boundary motion and pinning.

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MS85
Coverage Statistics for Sequence Census Methods

I will illustrate how to view fragments produced in a high-throughput sequencing experiment as a set of discrete points in the plane. This collection of points forms a two-dimensional spatial Poisson process, which yields a null model for random fragment coverage. After giving an overview of this model, I will show how the successive jumps of the depth coverage function can be encoded as a random tree. This discrete, probabilistic theory can potentially be of use in a wide variety of sequence census methods. Two specific applications will be presented: an algorithm for finding protein binding sites using ChIP-Seq data and a statistical test to address fragment bias in RNA-Seq data.

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MS85
Some New Combinatorial Problems from RNA

In the Fall of 2011, I taught a graduate-level topics course on Combinatorial Computational Biology of RNA. There were eleven grad students in the class, and they had diverse backgrounds and research areas. Our goal was to learn some of the mathematical results and techniques from the past decade and to pinpoint future research problems. In those regards, it was quite successful. I will summarize some of the main themes of the area as well as outline some new ideas and directions that a few graduate students from the class are currently pursuing in their research.

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MS85
Non-parametric Species Delimitation Based on Branching Rates

Many probabilistic tests have been developed to delimit species based on the coalescent model. These computational efforts rely primarily on parametric models that try to account for known variance found in genetic processes. Unfortunately, this variance is difficult to model precisely. Using non-parametric tests, we develop a method to delineate species by estimating the time species change from growth (e.g., Yule models) to a coalescence process without constraining the processes to a particular model. Using simulated gene trees from a known species tree, we compare our non-parametric method to established parametric methods.

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MS85
Reverse Engineering of Regulatory Networks Using Algebraic Geometry

Discrete models have been used successfully in modeling biological processes such as gene regulatory networks. When certain regulation mechanisms are unknown it is important to be able to identify the best model with the available data. In this context, reverse engineering of finite dynamical systems from partial information is an important problem. In this talk we will present a framework and algorithm to reverse engineer the possible wiring diagrams of a finite dynamical system from data. The algorithm consists on using an ideal of polynomials to encode all possible wiring diagrams, and choose those that are minimal using the primary decomposition. We will also show that these results can be applied to reverse engineer continuous dynamical systems.

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MS86

Acceleration of a Multiple Scattering High Frequency Iterative Method

A recent high frequency analysis of the Neumann series in the context of multiple scattering configurations shows that the rate of convergence converges to 1 when the distance separating scatterers converge to 0. This impairs the Krylov-subspace based iterative method that was designed especially to deal with this kind of problems. We propose a preconditioner based on the Kirchhoff approximation to improve this iterative solver.

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MS86

A Fast Iterative Method for Solving the Eikonal Equation on Triangular and Tetrahedral Domains using GPUs

In this talk we presents an efficient, fine-grained parallel algorithm for solving the Eikonal equation on unstructured triangular and tetrahedral meshes. The Eikonal equation, and the broader class of Hamilton-Jacobi equations to which it belongs, have a wide range of applications from geometric optics and seismology to biological modeling and analysis of geometry and images. The ability to solve such equations accurately and efficiently provides new capabilities for constructing solutions on large grids, exploring and visualizing parameter spaces, and for solving inverse problems that rely on such equations in the forward model. Efficient solvers on state-of-the-art, parallel architectures require new algorithms that are not, in many cases, optimal, but are better suited to synchronous updates of the solution and constrained memory access patterns. In this talk we address some particular challenges associated with 2D and 3D unstructured meshes, in order to extend the fast iterative method to solve the Eikonal equation efficiently on two-dimensional triangular and three-dimensional tetrahedral domains on parallel architectures, including graphics processors. We propose a new local update scheme which provides solutions of first-order accuracy on both serial and parallel architectures, and extend that scheme to the case of inhomogeneous, anisotropic speed functions. We also propose two novel update schemes and their corresponding data structures for efficient irregular data mapping to parallel, SIMD processors. We provide detailed descriptions of the implementations on a single CPU, a multicore CPU with shared memory, and SIMD architectures, with comparative results against state-of-the-art Eikonal solvers.

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MS86

High Frequency Wave Propagation with Geometrical Optics and Beyond

We propose a new method by combining the geometrical optics and Huygens-Kirchhoff identities to numerically solve the Helmholtz equation with single point-source condition in high frequency regime. Data compression with Chebyshev expansions and random sampling based pseudoskeleton approximations are applied to make the wavefield reconstruction efficient. The new approach is efficient and has no pollution effects. And it can reconstruct wavefields for a set of source points and a band of high frequencies.

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MS86

Efficient Computation of the Semi-Classical Limit of the Schroedinger Equation

An efficient method for simulating the Schroedinger equation near the semiclassical limit is presented. It uses a transformation based on Gaussian wave packets and yields a Schroedinger type equation ammenable to computation in the semi-classical limit. The number of grid points needed is small enough that computations in dimensions of up to 4 or 5 are feasible without the use of any basis thinning procedures. This is joint work with Giovanni Russo.

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MS87

Discretization of Integral Operators on Complicated Surfaces

I will describe an efficient method for the numerical evaluation of the singular integrals which arise in the discretization of weakly singular integral operators on surfaces. Standard techniques for evaluating these integrals, while adequate in simple cases, become prohibitively expensive when applied to integral operators given on complicated surfaces. The scheme I will describe, by contrast, is largely insensitive to the geometry of the underlying surface.

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MS87

Integral Equation Methods for Unsteady Stokes Flow in Two Dimensions

We present an integral equation formulation for the unsteady Stokes equations in two dimensions. This problem is of interest in its own right, as a model for slow viscous flow, but perhaps more importantly, as an ingredient in the solution of the full, incompressible Navier-Stokes equations. Using the unsteady Green's function, the velocity evolves analytically as a divergence-free vector field. This avoids the need for either the solution of coupled field equations (as in fully implicit PDE-based marching schemes) or the projection of the velocity field onto a divergence free field at each time step (as in operator splitting methods). In addition to discussing the analytic properties of the operators that arise in the integral formulation, we describe a family of high-order accurate numerical schemes and illustrate their performance with several examples.

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MS87
Boundary Integral Methods for Inextensible Vesicle Dynamics in Two Dimensions

A boundary integral method for simulating inextensible vesicles in a 2D viscous fluid was developed by Veerapaneni et. al. Recent extensions include developing preconditioners, implementing a near-singular integration strategy, allowing for vesicles with different bending moduli, and incoporating the Fast Multipole Method. The goal is to develop a robust method to simulate high concentrations of vesicles.

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MS87
Fast, High-order Accurate Methods for Evaluating Layer Heat Potentials

We will describe a new fast algorithm for evolving the "history part" of the heat potentials. It overcomes some of the limitations of previous fast algorithms and lowers the complexity constants. We will also discuss a new recursive product integration to overcome the "geometrically induced stiffness" of the heat potentials. The new scheme is arbitrary-order accurate and in particular, we present results that exhibit 16th order convergence for evaluating layer potentials on time-dependent boundaries. This is joint work with Lesle Greengard, Shidong Jiang and George Biros.

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MS88
Modeling Tear Films, Contact Lenses and Evaporation

We explore thin film models for the tear film on a human eye in the presence of a porous contact lens. We are interested in pre-lens and post-lens tear film dynamics. Our model assumes that the contact lens remains wetted upon evaporation of the pre-lens tear film and allows for continued evaporation from an exposed contact lens. Treatment of the post-lens film as a squeeze layer is also discussed.

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MS88
A Comparison of Numerical Methods for Models of Thin Liquid Films

Together, experiments, analytical solutions and numerical simulations have advanced our fundamental understanding of the motion of thin liquid films. The models involve partial differential equations that are tractable by several numerical approaches; there is no agreed-upon best scheme. Many mathematicians write their own code for numerical simulations. Open source code is uncommon. I will review pros and cons of a variety of numerical approaches to thin films problems and discuss possibilities for open source code.

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MS88
Settling of a Contact Lens

When a contact lens is placed in the eye, it is fit onto the cornea by the action of the blink. The upper lid applies a normal force on the lens deforming it and squeezing the tear film out between the lens and cornea. To better understand the fit performance, we model coupled fluid and solid mechanics of the settling of a soft contact lens during a blink.

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MS88
New Models of Two-phase Flow in Porous Media

Plane waves for two phase flow in a porous medium are modeled by the one-dimensional Buckley-Leverett equation, a scalar conservation law. We analyze stability of sharp planar interfaces to two-dimensional perturbations, which involves a system of partial differential equations. Linear stability analysis results in a criterion that distinguishes between stable and unstable interfaces. Numerical simulations of the full nonlinear system of equations, including dissipation and dispersion, illustrate the analytical results.

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MS89

Approximation on Non-Cartesian Lattices

For applications such as visualization in higher dimensions non-Cartesian uniform lattices outperform the Cartesian lattice. I will present a generic framework that extends popular approximation methods, such as B-splines, from the Cartesian lattice to uniform non-Cartesian lattices.

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MS89

Box-Splines on Crystallographic Lattices

The talk characterizes families of symmetric box-splines that are natural analogues of tensor-product B-splines, but that are shift-invariant on other crystallographic lattices that appear in nature, such as the BCC and FCC lattices and their generalizations. In particular, the talk summarizes the basic properties for computational use: the polynomial degree, the continuity, the linear independence of shifts on the lattice and optimal quasi-interpolants for fast approximation of fields.

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MS89

Patterns in Free Form Architecture and Discrete Differential Geometry

Contemporary architecture generates a stunning variety of new designs and patterns which are based on freeform geometry. These patterns are often closely related to the actual fabrication, for example in panel layouts and supporting structures. In this talk, the speaker will address the mathematical concepts behind some recent developments, which are closely linked to discrete differential geometry and concern circle patterns, geodesic patterns and patterns formed by support structures and shading systems.

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MS89

Shape Space Exploration of Constrained Meshes

In geometry processing, meshes are often specified by a collection of non-linear constraints, typically associated with mesh faces or edges. Exploring the corresponding shape space, i.e., the possible meshes sharing the same combinatorics while satisfying the constraints, are widely believed to be challenging. In this talk, I will present a general method to locally characterize any shape space of meshes implicitly prescribed by a collection of non-linear constraints and how to navigate the desirable subspaces.

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MS90

Learning to Classify HSI

We present a sparse modeling framework for sub-pixel mapping that mitigates the effects of noise, spectral variability, and spectral mixing by learning material dictionaries, and a spatialspectral coherence regularizer. Experiments with synthetic and real data demonstrate the suitability of the method. This technique retains high-performance classification accuracy when dealing with reconstructed data from undersampled images. Finally, we apply this technique for HSI-LiDAR fusion. Work in collaboration with Zhengming Xing, John Greer, Edward Bosch, and Lawrence Carin.

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MS90

Classification of Hyperspectral Images by Variational Methods

Hyperspectral classification methods have often focused on the wealth of spectral information available in each pixel. However, the incorporation of spatial information can also greatly aid in object identification. We will discuss the adaptation of variational segmentation methods, primarily designed for grayscale and color imagery, to the segmentation of hyperspectral data. We also show that multi-phase segmentation finds a natural extension into the high dimensions of hyperspectral data.

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MS90

Social Network Clustering of High Dimensional Sparse Data

Data mining is the mathematics, methodologies and procedures used to extract knowledge from large datasets. Spectral embedding uses eigenfunctions of a Laplace operator (or related graph affinity matrix) for extracting the underlying global structure of a dataset. This talk will give an introduction to spectral embeddings. Applications presented will include clustering LA street gang members based on sparse observations of where and who they are seen with.

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MS90

Robust Computation of Linear Models

Consider a dataset of vector-valued observations that consists of a modest number of noisy inliers, which are explained well by a low-dimensional subspace, along with a large number of outliers, which have no linear structure. We describe a convex optimization problem that can reliably fit a low-dimensional model to this type of data. When the inliers are contained in a low-dimensional subspace we provide a rigorous theory that describes when this optimization can recover the subspace exactly. We also formulate an efficient algorithm for solving this optimization problem and demonstrate its effectiveness with numerical experiments.

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MS91

Determinants of Successful Cancer Therapy with Cytokine-expressing Oncolytic Viruses

Oncolytic viruses selectively infect and destroy tumors while largely sparing healthy cells. Many of today's most promising oncolytic viruses express cytokines which induce an immune attack against the tumor. Here, we systematically develop deterministic mathematical models describing the therapeutic mechanism. For model validation, we leverage *in vivo* measurements illustrating the antitumor effects of several cytokine-armed oncolytic adenoviruses in melanoma cells. We present our modeling approach and preliminary findings regarding the mathematical basis for tumor elimination.

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MS91

The Role of Biomechanics in the Early Development of Breast Cancer: A Hybrid Model

We investigated the role of microenvironment in an early development of Ductal carcinoma in situ (DCIS) and the invasion process in later stages. DCIS is an early stage noninvasive breast cancer that originates in the epithelial lining of the milk ducts, but it can evolve into comedo DCIS and ultimately the most common type of breast cancer, invasive ductal carcinoma. Understanding the progression and how to effectively intervene in it presents a major scientific challenge. The extracellular matrix (ECM) surrounding a DCIS tumor contains several types of cells and several types of growth factors that are known to individually affect tumor growth. However, the complex biochemical and mechanical interactions of stromal cells with tumor cells is poorly understood. The model can predict how perturbations of the local biochemical and mechanical state influence tumor evolution via cross-talk between a tumor and stromal cells such as fibroblasts. We first focus on the EGF-TGFbeta signaling pathways and show how cell growth and proliferation can be affected by up- or down-regulation of components in these pathways. We present a hybrid model for the interaction of cells with the tumor microenvironment (TME), in which epithelial cells (ECs) are modeled individually while the ECM is treated as a continuum, and show how these interactions affect the early development of tumors. We then present an invasion model where stromal cells play a significant role in triggering the invasion process. Our results shed light on the interactions between growth factors, mechanical properties of the ECM, and feedback signaling loops between stromal and tumor cells, and suggest how epigenetic changes in transformed cells affect tumor progression in the early and late stage of breast cancer.

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MS91

Modeling Preventative Breast Cancer Vaccines using an Agent-based Approach

A next generation approach to breast cancer treatment focuses on developing preventative vaccinations to stimulate a person's immune system to attack incipient tumors before clinical detection. Relevant cell interactions would take place on the scale of several thousands of cancer cells. To understand dynamics at this small scale, we develop an agent-based model of anti-tumor immune responses that accounts for cell size, cell crowding near the microtumor, and the possibility of stochastic tumor elimination.

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MS91

Traveling Waves in a Model of Tumor Angiogenesis

In this talk, we will discuss traveling wave solutions for a chemotaxis model with logarithmic sensitivity, which describes the initiation of angiogenesis. The challenges of analyzing traveling wave solutions of such type of chemotaxis model lie in the high dimensionality and the singularity. Hence the routine approaches, such as phase plane analysis, no longer work. In the talk, we shall show these challenges can be resolved by variable transformations,such that the transformed system can be solved by the regular approaches. The existence, wave speed and stability of traveling wave solutions will be discussed and open questions will be presented.

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MS92

The Extended Combinatorial Inverse Eigenvalue Problem

Let $\mathcal{S}(\mathcal{G})$ be the set of all real symmetric $n \times n$ matrices corresponding to a graph G on n vertices. We investigate the problemGiven G, a vertex v of G, and $2n-1$ real numbers

$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n,$$

is there a matrix $A \in \mathcal{S}(\mathcal{G})$ such that $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of A and $\mu_1, \ldots, \mu_{n-1}$ are the eigenvalues of $A(v)$?A complete solution can be found for a few graphs on n vertices.

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MS92

Zero Forcing, Minimum Rank, and Applications to Control of Quantum Systems

We study the dynamics of systems on networks from a linear algebraic perspective. Under appropriate conditions, there is a connection between the quantum (Lie theoretic) property of controllability and the linear systems (Kalman) controllability condition. We investigate how the graph theoretic concept of a zero forcing set impacts the controllability property. In particular, we prove that if a set of vertices is a zero forcing set, the associated dynamical system is controllable. Joint work with Burgarth, DAlessandro, Severini, Young.

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MS92

Lower Bounds for Minimum Semidefinite Rank

The minimum semidefinite rank (msr) of a graph is the minimum rank among positive semidefinite matrices with the given graph. The OS-number is a useful lower bound for msr, which arises by considering ordered vertex sets with some connectivity properties. In this talk we present two new interpretations of the OS-number. We first show that OS-number is also equal to the maximum number of vertices which can be orthogonally removed from a graph under certain nondegeneracy conditions. Our second interpretation of the OS-number is as the maximum possible rank of chordal supergraphs who exhibit a notion of connectivity we call isolation-preserving. These interpretations not only give insight into the OS-number, but also allow us to prove some new results. For example we show that $msr(G) = |G| - 2$ if and only if $OS(G) = |G| - 2$.

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MS92

Positive Semidefinite Zero Forcing

The positive semidefinite zero forcing number of a graph, $Z_+(G)$, is a variant of the (standard) zero forcing number of a graph, $Z(G)$, which uses the same definition with a different color change rule. The positive semidefinite zero forcing number was introduced as an upper bound for positive semidefinite maximum nullity. This talk will discuss properties of $Z_+(G)$ and positive semidefinite zero forcing sets. Joint work with Ekstrand, Erickson, Hall, Hay, Hogben, Johnson, Kingsley, Osborne, Peters, Roat, Ross, Row, Warnberg.

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MS93

Assessing Beliefs and Content Knowledge in First Semester Biocalculus

Many colleges and universities struggle with finding ways to meet the quantitative needs of their biology and life science majors. Here I will share my experiences in the development and implementation of a first semester calculus course for biology majors. I will discuss assessment of student beliefs and attitudes about mathematics pre- and post-biocalculus, their performance as compared to students in traditional calculus, and the similarities and differences in their styles of learning mathematics.

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MS93

Calculus II for Biology Students

Abstract not available at time of publication.

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MS93

Introducing Quantitative Thinking into an Introductory Biology Curriculum

Introducing quantitative thinking in introductory biology classes presents challenges from students and instructors. To address these, we have identified quantitative concepts that support introductory biology concepts; designed tutorials and exercises placing them in biological contexts; designed an instrument to assess the effectiveness of this approach; and piloted the approach in a small section of introductory biology. This work is supported by a grant to the University of Arizona from the Howard Hughes Medical Institute (52006942).

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MS93

A New Quantitative Modeling Course for First-year Biology Students

In the last few decades biological and medical fields have undergone a profound transformation into data-driven, quantitative sciences. The standard calculus courses which traditionally constitute the quantitative training for biology majors do not adequately prepare students for these needs. A new course developed at the University of Chicago takes the place of the last course in the required calculus sequence. It combines mathematical modeling, computational implementation, and basic statistics, all applied to specific biological and medical problems. I will present the results of assessments, both of student learning and of their evaluations of the course effectiveness.

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MS94

Multi-precision Inner/outer Solvers via Generic Programming Libraries

Multi-precision and mixed-precision techniques combine inefficient high-precision types with efficient low-precision types in order to provide fast and high-precision solvers and preconditioners. Traditional approaches typically utilize a high precision solver preconditioned using a lower precision solve, but modern generic programming techniques allow researchers and pracitioners a rich set of possibilities, including deep recursive solves and mixed-precision primitives. We demonstrate hybrid-parallel multi-precision iterative linear and eigenvalue solvers using the generic programming library support in Trilinos.

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MS94

Design and Development of Sustainable Libraries for Numerical Computation on Many Core Architectures

The new supercomputers have millions of cores interconnected hierarchically by high-speed networks. The hierarchic and massive parallelism present in these architectures imply that the numerical libraries have to be defined according to an adequate design model and the existing ones would have to be adapted to this design. In this talk, we present a model for numerical library allowing reusability and sustainability. Some experiments on large scale many-core platforms validating the approach will be presented.

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MS94

Incorporation of Multicore FEM Integration Routines into Scientific Libraries

We have developed a system for integration of the finite element residual and Jacobian arising from a given weak form. This system is based upon the Ignition code generation package and ideas from the FEniCS project, and generates code targeting GPUs. Since this is merely a part of the overall PETSc library framework, we discuss the design decisions made in order to incorporate these routines with a minimum of user input, generation of debuggable code, and smooth integration into the PETSc build process.

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MS94

Cray Scientific Library for Accelerators

We will present Cray Scientific Libray for accelerators designed for Cray XK family. This library provides the same interface of the original BLAS and LAPACK that can be executed on accelerators and CPUs together. For the performance enhancement, we have applied an auto-adaptation mechanism to select the best implementation for different problem size, type of host memory allocation and data location. These features deliver immediate speed up for existing applications with relatively light coding efforts.

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MS95

Resilience of Small Social Networks with Multiple Relations

The ability of a network to retain a given property under perturbation of its structure is referred to as *resilience*. We focus on the resilience of small social networks with multiple types of relations. Here, we describe the multirelational structure as a partially ordered semigroup, represented by its Hasse diagram. We discuss qualitative differences between networks with connected and disconnected Hasse diagrams, and we illustrate the resilience formulation with a number of empirical examples.

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MS95

Matroidal Branchwidth

Abstract not available at time of publication.

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MS95

Price Optimization under the Nested Logit Model With Multiple No-Purchase Options

We consider a pricing problem under the Nested Logit Model in which nests represent agencies acting as amalgamators of product offerings from several firms, rather than being wholly controlled by a single firm. We consider a revenue maximization problem from the perspective of a single firm utilizing n channels and show that the optimal revenue can be obtained by an iterative procedure which adjusts prices sequentially over each nest.

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MS95

Optimal Toll Design: A Lower Bound Framework for the Traveling Salesman Problem

We propose a framework of lower bounds for the asymmetric traveling salesman problem based on approximating the dynamic programming formulation, and give an economic interpretation wherein the salesman must pay tolls as he travels between cities. We then introduce an exact reformulation that generates a family of successively tighter lower bounds, all solvable in polynomial time, and compare these new bounds to the well-known Held-Karp bound.

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MS96

Eulerian Approaches for Transmission Traveltime Tomography with Discontinuous Slowness

We propose an Eulerian approach for transmission traveltime tomography with discontinuous slowness. The approach is to minimize the mismatch between the measurements and the Eulerian solutions of the eikonal equation. To accurately incorporate the contributions from discontinuity in the slowness, we propose a level-set formulation to describe the discontinuity in the velocity model. This results in a shape recovery problem. In the first part of the talk, we match only the first arrivals from point sources. Even though the algorithm is computationally efficient, such approach discards all information from later arrivals. In the second part of the talk, we consider using multivalued Eulerian traveltime solutions. We propose a novel algorithm to compute such multivalued solutions of the eikonal equation without doing any computation in the phase space. Preliminary numerical results will also be given.

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MS96

Simulation of Light Waves in Large Scale Photonic Crystal Devices

Photonic crystals (PhCs) are periodic structures with a period on the scale of the wavelength of light. Devices can be created in a PhC by introducing various types of defects and they are usually connected by waveguides that serve as input and output ports. A large scale PhC device may have a length scale that is much larger than the wavelength. We present some techniques for simulating lightwaves in PhC devices. These techniques can take advantage of the existence of many identical unit cells, the partial periodicity of the structure and the locality of some nonlinear processes, etc.

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MS96

Unformization of WKB Solutions via Wigner Transform

We propose a renormalization process of a two phase WKB solution, which is based on an appropriate surgery of local uniform asymptotic approximations of the Wigner transform of the WKB solution. We explain in details how this process provides the correct spatial variation and frequency scales of the wave field on the caustics where WKB method fails. The detailed analysis is presented in the case of a fundamental problem, that is the semiclassical Airy equation, which arises from the model problem of acoustic propagation in a layer with linear variation of the sound speed.

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MS96

Randomized Structured Direct Solvers for Seismic Problems

We consider the solution of 2D and 3D inhomogeneous acoustic wave equation in the frequency domain, by solving Helmholtz equations via a new set of structured matrix methods. Randomized techniques are used to facilitate the structured matrix operations. The advantages of such solvers include: 1. For a single frequency, all solution steps share a common Helmholtz operator, which can be quickly factorized so as to solve linear systems with multiple right-hand sides, each in nearly linear time and storage. We take advantage of certain hidden rank structures in the operators. 2. For different frequencies, the same adjacency pattern is used, so that only one step of matrix ordering is needed. 3. The factorizations are relatively insensitive to the frequencies. We try to justify such insensitivity. The efficiency and accuracy are demonstrated by various important numerical examples, such as 2D (BP2004 & BP2007 TTI) and 3D (SEAM) models. This is joint work with Maarten V. de Hoop, Xiaoye S. Li, and Shen Wang.

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MS97

Fast Computation of Eigenfrequencies of Planar Domains via the Spectrum of the Neumann-to-Dirichlet Map

We present a new method for the spectrum and eigenfunctions of a planar star-shaped Dirichlet domain. It is 'fast' since it is computes a *cluster* of eigenfunctions (numbering of order the square-root of the eigenvalue) with the effort usually taken to find a *single* one. For a domain 400 wavelengths across, and relative error 10^{-10}, the resulting speed-up is $\sim 10^3$. Its error analysis is rigorous, and it achieves higher-order accuracy than the 'scaling method'. I will also discuss a new technique for evaluation of potential fields close to their source curves.

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MS97

A Fast Direct Solver for Non-oscillatory Integral Equations

We present a fast direct solver for non-oscillatory integral equations via multilevel matrix compression and sparse matrix embedding. For boundary integral equations in 2D, the solver has optimal $\mathcal{O}(\mathcal{N})$ complexity, where N is the system size; in 3D, it incurs an $\mathcal{O}(\mathcal{N}^{\ni/\in})$ precomputation cost, followed by $\mathcal{O}(\mathcal{N}\log\mathcal{N})$ solves. Numerical experiments suggest the utility of our method as a direct solver, a generalized fast multipole method, and as a preconditioner for complex problems.

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MS97

Fast Methods for Boundary Integral Equations on the Sphere

Models describing physical or biological phenomena constrained to evolve on subsurfaces of compact manifolds can be reformulated in terms of integral equations. Examples of such models include point vortices moving on the surface of the earth, or polar-driven chemotactic migration on cell membranes during mitosis. The use of integral equation strategies in this context is fairly new, and requires a careful examination of the relevant parametrices for the elliptic operator of concern. In this talk we first describe reformulations of a boundary value problem for the Laplace-Beltrami operator in terms of layer potentials. We then describe a class of fast methods based on the fast multipole method.

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MS97

Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver

We present recent progress on the development of the adaptive fast multipole Poisson-Boltzmann solver. We briefly review previous efforts on integral equation reformulation, mesh generation and discretization, and new versions of the fast multipole methods. We introduce our recent progress on parallelization based on the dynamic prioritization technique for large-scale problems and on-going work on time-marching schemes for long-time simulations.

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MS98

Undergraduate Research on the Fast Track: From Nothing to Publication in Eight Weeks

Since Summer 2010, we have been hosting the REU Site: Interdisciplinary Program in High Performance Computing. It introduces undergraduate students to scientific, statistical, and parallel computing with MPI and conducts research with application scientists from industry, academia, and government agencies in only eight weeks. We will share our experiences of how to make this program work through team work and by involving several layers of support from graduate students to faculty, with lessons that are useful for anyone interested in running an REU Site.

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MS98

Building An Applied and Computational Math Degree Program from the Ground Up

We are developing a new undergraduate degree program in applied and computational mathematics, scheduled to commence Fall 2013. Each year, this major will admit a cohort of up to 40 students into a two-year lock-step curriculum commencing at the beginning of their junior year and continuing through to graduation. This carefully planned educational experience will provide students with a tightly integrated combination of coursework and computer labs, together with a capstone project and close mentoring.

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MS98

Models for Undergraduate Research, Best Practices, and Questions

This talk will highlight some successful models that faculty have used to foster undergraduate research, some best practices that have emerged, and some questions that remain.

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MS98

Multidisciplinary Undergraduate Research in Computational Mathematics and Nonlinear Dynamics of Biological, Bio-inspired and Engineering Systems

In this talk, we will describe a multidisciplinary undergraduate research program in computational mathematics and nonlinear dynamics of biological, bio-inspired and engineering systems that has not only helped to enhance ongoing interaction among communities of people including students, educators and academicians, but also serve as a catalyst to help reinforce and drive reform across the institution.

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MS99

Mapping the Connectome with Convex Algebraic Geometry

The human brain connectome project seeks to provide a complete map of neural connectivity. Just as the human genome represents a triumph of marrying technology (high throughput sequencers) with theory (dynamic programming for sequence alignment), the human connectome is the result of a similar union. The technology is that of diffusion magnetic resonance imaging while the requisite theory, we shall argue, comes from a combination of harmonic analysis and convex algebraic geometry.

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MS99

Klein's Idea and Identities for Powers of Polynomials

In his famous book on the icosahedron, Felix Klein considered the identification of a point on the unit sphere u, with the linear form $x - vy$, where v is the image of u under the Riemann map. If you start with the vertices of a nice polytope inscribed in the sphere, and take quadratic forms corresponding to products of linear forms associated with antipodal pairs of vertices, you get interesting sets of quadratic forms. For example, the octahedron corresponds to $xy, x^2 - y^2, x^2 + y^2$ (the Pythagorean parameterization), the cube to four quadratic forms whose 5-th powers are dependent and the icosahedron to six quadratic forms whose 14-th powers are dependent. We'll give more examples and try to explain this phenomenon.

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MS99
Linearization Functors on Real Convex Sets

We prove that linearizing certain families of polynomial optimization problems leads to new functorial operations in real convex sets. We show that under some conditions these operations can be computed or approximated in ways amenable to efficient computation. These operations are convex analogues of Hom functors, tensor products, symmetric powers, exterior powers and general Schur functors on vector spaces and lead to novel constructions even for polyhedra.

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MS99
A Sums of Squares Relaxation for Hyperbolicity Cones

Hyperbolic programming a useful generalization of semidefinite programming. Here we will investigate the relationship between them. Using derivative cones, I will give an inner approximation of a hyperbolicity cone using sums of squares. In particular, this will give an inner approximation of the hyperbolicity cone by the feasible set of an SDP. As a bonus, this relaxation is exact for hyperbolic polynomials already coming from an SDP.

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MS100
Spline Operators for Subdivision and Differentiation

The discrete derivatives of a Bezier curve are known to converge to the continuous derivative under subdivision. So after a sufficient number of subdivisions one can obtain a 'good' approximation of the derivative. Here a tight error bound for this approximation is derived and the number of subdivisions required for a prescribed error tolerance is calculated. This is done considering the subdivision algorithm as an operator acting on the control points of the curve.

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MS100
The Case Against Interactivity in Geometric Design

Interactive geometric design tools are now a firmly entrenched means of building geometric models suitable for product definition and engineering analysis. Such tools have seemingly been a boon to mechanical engineering and product design worldwide, and it is hard to imagine a modern design shop in which such tools don't play a vital role.

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MS100
Knot Theorems and Counterexamples for Splines

For piecewise linear approximation of spline curves, it is well-known that repeated subdivision produces a control polygon that converges to the spline under the Hausdorff metric. Little has been shown about the relationship of topological properties between the control polygon and its spline curve. We i) provide sufficient conditions for subdivision to yield a control polygon ambient isotopic to the curve, and ii) show examples of topological differences between a spline and its control polygon.

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MS100
Volume Rendering Verification Using Discretization Errors Analysis

Much recent research has been dedicated to direct volume rendering (DVR). In disciplines such as image-based medical diagnosis or material science, images generated using DVR require high accuracy and precision. Unfortunately, little research has been dedicated to assess volume rendering correctness. We propose a technique for volume rendering verification based on an analysis of the volume rendering integral. We apply order-of-accuracy and convergence analysis - well-established verification techniques - to volume rendering implementations, and derive the theoretical foundations of our verification approach.

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MS101
Non-modal Amplification of Disturbances in Channel Flows of Viscoelastic Fluids: A Possible Route to Elastic Turbulence?

Abstract not available at time of publication.

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MS101
Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS101
Regularized Two-phase Models for Gels

Abstract not available at time of publication.

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MS102
2-Matching Covered Loopy Graphs

A $\{1, 2\}$-factor is a spanning subgraph consisting of pairwise vertex disjoint edges and cycles. Tutte has characterized graphs which have a $\{1, 2\}$-factor. We investigate minimal 2-matching covered graphs, i.e. graphs in which every edge is in some $\{1, 2\}$-factor and removal of any edge yields a graph without this property. We will discuss some classes of minimally 2-matching covered loopy graphs (graphs in which vertices may have a loop), where loops are cycle of length one.

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MS102
Spectrally Arbitrary Patterns over Finite Fields

A zero-nonzero pattern is a square matrix where each entry is either a zero or a star. A realization of a zero-nonzero pattern over a specified field is a matrix where each of the stars is replaced by a nonzero entry from the field. A pattern is said to be a Spectrally Arbitrary Pattern over the specified field if for every monic polynomial(with degree corresponding to the size of the matrix) with coefficients from the field, there exists a realization whose characteristic polynomial is the given polynomial. We will look at the interplay between pattern structure and field stucture in determining whether or not a pattern turns out to be spectrally arbitrary over a given field.

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MS102
Minor Monotone Floors and Ceilings of Graph Parameters

A graph parameter is minor monotone if it preserves the minor relation. We consider the transformation of real-valued graph parameters into related minor monotone graph parameters using two different methods. The minor monotone floor of well-ordered graph parameter p is defined by $\lfloor p \rfloor = \min\{p(H) | G \preceq H\}$ with a similar definition for the minor monotone ceiling. We consider the minor-monotone floor and ceiling of a number of graph parameters, with particular attention given to parameters that relate to the zero-forcing number. Results dealing with the Hadwiger conjecture are also considered.

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MS102
A Colin de Verdiere-type Invariant and odd-K_4- and odd-K_3^2-free Signed Graphs

A signed graph is a pair (G, Σ) where G is an undirected graph (we allow parallel edges, but no loops) and $\Sigma \subseteq E(G)$. A cycle C of G is called odd if C has an odd number of edges in common with Σ. A signed graph is called bipartite if it has no odd cycles. We have introduced $\nu(G, \Sigma)$, which generalizes the Colin de Verdière invariant $\nu(G)$. The invariant ν characterizes bipartite signed graphs as those signed graphs (G, Σ) with $\nu(G, \Sigma) \leq 1$, and signed graphs with no odd-K_4- and no odd-K_3^2-minor as those signed graphs (G, Σ) with $\nu(G, \Sigma) \leq 2$. In this talk we will discuss these results. Joint work with Marina Arav, Frank Hall, and Zhongshan Li.

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MS103
Dynamic Density Functional Theory (DDFT) Model for Freezing of a Pair Potential Fluid: The Effect of Fluid Flow

The Classical Density Functional Theory (CDFT) and the Phase Field Crystal (PFC) models have proven to be good approaches to model crystal growth from a fluid phase. These models capture atomic level details including defects and grain boundaries. However these approaches usually involve a phenomenological gradient descent based time evolution. and do not take the convection of the fluid phase (fluid flow) into consideration. In this work we start with the Revised Enskog Theory (RET) (an effective kinetic theory) as the definition of time evolution. Then exploiting the connection to CDFT of freezing, we develop evolution equations for the macroscopic density and flow fields. The over damped limit provides us a DDFT model for time evolution of the density field. Some studies of this model and results on crystal growth from fluid phase will be discussed.

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MS103
Liquid Crystal Phase Transitions in Elastic Net-

works

We develop a modelling approach to anisotropic, nonlinear elasticity using ideas from the liquid crystal theory. We consider highly compressible elastic networks with embedded rigid units. The work is motivated by the structure and functionality of actin and collagen networks found in inter-connective tissue. We analyze the phase transition behavior of these systems under compression and shear, and found a range of nematic phases and a soft-elasticity regime, according to geometric properties of the network.

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MS103

A General Framework for High Accuracy Solutions to Energy Gradient Flows from Material Science Models

Abstract not available at time of publication.

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MS103

Energy Stable Scheme for Phase Field Models

Abstract not available at time of publication.

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MS104

Nucleation Events in Soft Condensed Matter Using the String Method

Within the self-consistent field theory, we develop an "on-the-fly' string method to compute nucleation events in soft-condensed matter systems. Several applications of the method are given, including: membrane pore formation and rupture, particle translocation, and the budding of a micelle from a rod-like micelle. Where applicable, the method is compared against classical nucleation theory.

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MS104

Failure of Random Materials: Asymptotic Analysis and Importance Sampling

We study the problem of estimating small failure probabilities for elastic random material which is described by a one dimensional stochastic elliptic partial differential equation with certain external force and boundary conditions. Gaussian random function is used to model the spatial variation of the material property parameters. The failure event of the bulk material is simply characterized by the exceeding of certain thresholds for the max stress or load in any spatial location. With the large deviation heuristics, we provide a intuitive description of the most probable realization of the random material parameters which could lead to the critical situation of material failure in engineering. An efficient Monte Carlo method to compute such probabilities is presented.

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MS104

Sampling Transition States Using Gentlest Ascent Dynamics

The dynamics of complex systems often involve thermally activated barrier-crossing events that allow the system to move from one basin of attraction on the energy surface to another. Such events are ubiquitous, but difficult to simulate using conventional simulation tools like molecular dynamics. We present an extension of the gentlest ascent dynamics (GAD) under which the system evolves in a manner opposite to that of the steepest descent method.

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MS104

Some Interacting Particle Methods for Sampling Complex Energy Landscapes

This talk will survey my efforts with coworkers to develop and analyze Monte Carlo sampling algorithms for complex (usually high dimensional) probability distributions. These sampling problems are typically di?cult because they have multiple high probability regions separated by low probability regions and/or they are badly scaled in the sense that there are strong unknown relationships between variables. The dimensionality and complexity of the problems necessitate a Monte Carlo approach (as opposed to numerical quadrature) but standard MC schemes converge extremely slowly in the presence of barriers or bad scalings. New methods designed to address these issues directly have the potential to significantly accelerate the solution of important problems in many areas of science. I'll discuss some very preliminary work on geophysical and chemical applications.

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MS105

Parametric Steering for Autotuning Numerical Kernels and Scientific Codes in Multicore Environments

Our goal is to find a way to represent the correlation between different performance tuning parameters, autotuning techniques and understand their relevance for implementing different numerical kernels in multicore environments. Our goals are to find some trends in performance driving parameters and form a criteria for the case-based selection of kernels at runtime.

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MS105

Promise Chaining for Automatic Kernel Fusion and Avoiding Data Movement on Accelerators

Performance optimizations for discrete compute accelerators (like GPUs) cut across computational kernels. For example, launching a single kernel is expensive, which motivates "fusing" multiple kernels. Moving data from the accelerator to the CPU is slow, which forces programmers to track data placement. Cross-kernel optimizations clutter interfaces, confuse algorithm developers, and hinder evolution of kernel optimizations. We propose a programming model that uses dataflow and promise chaining to hide data placement and fuse kernels automatically.

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MS105

Adaptation of ppOpen-AT To Numerical Kernels on Explicit Method

ppOpen-AT is an auto-tuning (AT) language for code optimization in 5 kinds of crucial numerical methods provided by ppOpen-HPC project. In this presentation, we present preliminary result by adapting ppOpen-AT to a numerical kernel derived by explicit method on Finite Difference Method. We have developed a new AT function on ppOpen-AT for its code optimization; loop fusion and loop split. Performance evaluation is performed by using the T2K Open Supercomputer (U.Tokyo) and HITACHI SR16000/M1.

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MS105

ppOpen-HPC: Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications with Automatic Tuning

ppOpen-HPC is an open source infrastructure for development and execution of optimized and reliable simulation codes with capabilities of automatic tuning (AT) on post-peta (pp) scale parallel computers using heterogeneous computing nodes which consist of multicore CPUs and co-processors. ppOpen-HPC consists of various types of libraries, which covers various types of procedures for scientific computations. In this talk, current status of ppOpen-HPC and results of recent developments are described.

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MS106

Self-assembly of Islands during the Initial Stages of Film Growth: Sizes and Spatial Arrangements

Atoms deposited on a flat surface at the onset of film growth diffuse and aggregate into islands (whose locations impact subsequent multilayer film morphologies). The size distribution and spatial arrangement of islands reflect the stochastic nature of the self-assembly process. Mean-field treatments fail to describe this behavior prompting development of alternative formalisms. We describe recent analysis for the distribution of capture zones, where the surface is tessellated so that one capture zone surrounds each island.

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MS106

On the Dynamics of Crystal Facets in Materials Surface Relaxation

Below the roughening temperature, crystal surfaces relax through the motion of line defects (steps); and develop macroscopically flat surface regions (facets). A challenging problem is to reconcile step motion, which is described by discrete schemes, with a viable continuum theory, based on variational principles and Partial Differential Equations, near facets. In this talk, I will discuss recent progress in formulating and analyzing an evaporation step model that is fully consistent with a continuum thermodynamics approach.

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MS106

Strain Dependence of Microscopic Parameters and its Effect on Ordering during Epitaxial Growth

Strain is often the driving force behind self-organization of quantum dots and other nanoscale structures. I present a DFT analysis of the effect of strain on key microscopic growth parameters. I then illustrate in growth simulations that employ the level-set technique how such strain dependence affects growth. This approach includes a variable (and strain dependent) potential energy surface for adatom diffusion, and an additional step-edge barrier via a mixed Robin boundary condition.

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MS106

Kinetic Monte Carlo Simulation of Heteroepitaxial Growth: Wetting Layers, Quantum Dots, Capping, and NanoRings

A KMC algorithm efficiently accounting for elastic strain is developed for heteroepitaxial growth. It exploits the observation that adatoms are essentially decoupled from the elastic field. The film is therefore decomposed into weakly and strongly bonded portions. The first evolves independent of the elastic field which is updated infrequently. We show that faceted quantum dots form from layer-by-layer nucleation of pre-pryamids. Capping simulations provide insights into dot erosion and ring formation. Joint with T.P. Schulze.

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MS107

Numerical Solution of An Inverse Diffraction Grating Problem

In this talk, we consider the diffraction of a time-harmonic plane wave incident on a perfectly reflecting periodic surface. A continuation method on the wavenumber will be proposed for the inverse diffraction grating problem, which reconstructs the grating profile from measured reflected waves on a constant height away from the structure. Numerical examples will be presented to show the validity and efficiency of the proposed method.

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MS107

Resoance of 1D Phototic Crystal with Finite Extent

Abstract not available at time of publication.

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MS107

Numerical Methods for the Complex Helmholtz Equation and Scattering from a Lossy Inclusion

I will discuss a new method for solving the Helmholtz equation in lossy materials that is based on the variational principles developed by Milton, Seppecher, and Bouchitté. This method results in a system of equations which can be reduced to a symmetric positive-definite system, and can be solved using conjugate gradient and Cholesky factorization. Also, I will discuss the application of this method to the problem of scattering from an inclusion filled with lossy material, which requires the application of a transparent boundary condition.

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MS107

Mathematical Analysis in Quantifying Mechanical Properties for Nano-Materials

Nanotechnology deals with structures sized between 1 to 100 nanometer and involves investigating and designing materials or devices within that scale. Due to its small size, it is difficult to quantify the mechanical properties of nanomaterials which significantly rely on measurement techniques, conditions and environment. In this talk, we propose a novel model based on Euler-Bernoulli equation with a stochastic source term accounting for the effect of initial bending, surface roughness and white noise during the measurement. The forward problem is demonstrated to have a unique and explicit path-wise solution. Furthermore, the inverse problem consists of identifying the elastic modulus of nanobelt and reconstructing the random source structure, i.e., the mean and the variance. Based on the explicit formula of the direct problem, the inverse problem can be reduced into a first kind of Fredholm type integral equation. Two kinds of regularization techniques are introduced to obtain stable solutions. Numerical examples are presented to illustrate the validity and effectiveness of the proposed methods.

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MS107

Phase Retrieval for Diffractive Imaging

Abstract not available at time of publication.

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MS108

Climate Transitions in a Conceptual Model with Multiple Time Scales

Techniques from dynamical systems are used to analyze a multiple timescale conceptual model incorporating temperature, glacial motion, and the carbon cycle. Within this framework, we examine how both ice-albedo and greenhouse gas feedback effects can cause a wide variety of glacial oscillations, including variations between ice-covered and ice-free states.

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MS108

A Dynamical Systems Perspective on Period Transitions in Glacial Cycles

About one million years ago, the Earth's glacial cycles changed character, increasing in amplitude and moving from a period of about 40 thousand years to a period of about 100 thousand years. Various theories attempting to explain this transition can be expressed as dynamical systems phenomena.

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MS108

Abrupt and Gradual Transitions from the Deep Past

Gaining information about ancient Earth climates is not an easy task. Then, once data is acquired, what insights can be gained? In this talk, we consider the observations and scientific hypothesis around two historic transitions in Earth's history. Approximately 650 million years ago, Earth is likely to have been completely covered in ice in what is called "Snowball Earth". Additionally we'll consider an abrupt transition (PETM) when atmospheric carbon sky rocketed nearly 55 million years ago.

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MS108

Climate Tipping Points: Overview and Outlook

I will provide some overview of investigations of potential tipping elements in Earths climate, highlighting challenges of developing early warning signs for impending critical transitions. Drawing on material covered in our "virtual seminar" on this topic, I will survey mathematical mechanisms for tipping, some of which depart from classical bifurcation theory. Parts of the discussion will be framed in terms of case studies associated with conceptual models of (1) Arctic sea-ice retreat, and (2) desertification.

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MS109

Optimality of the Neighbor Joining Algorithm and Faces of the Balanced Minimum Evolution Polytope

Balanced minimum evolution (BME) is a statistically consistent distance-based method to reconstruct a phylogenetic tree from an alignment of molecular data. In 2000, Pauplin showed that the BME method is equivalent to optimizing a linear functional over the BME polytope, the convex hull of the BME vectors obtained from Pauplins formula applied to all binary trees. The BME method is related to the popular Neighbor Joining (NJ) algorithm, now known to be a greedy optimization of the BME principle. In this talk I will elucidate some of the structure of the BME polytope and strengthen the connection between the BME method and NJ Algorithm. I will show that any subtree-prune-regraft move from a binary tree to another binary tree corresponds to an edge of the BME polytope. Moreover, I will describe an entire family of faces parametrized by disjoint clades. Finally, given a phylogenetic tree T, I will show that the BME cone and every NJ cone of T have intersection of positive measure.

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MS109

WNT Signaling in Melanoma Cells

Experimental evidence suggests that retinoic acid deactivates canonical WNT signaling in early stage melanoma cells, thereby affecting cell division. More agressive melanoma cell lines are not responsive to retinoic acid. The question then arises how such a switch in signaling could be affected in these unresponsive cell lines. This talk will discuss a time- and state-discrete mathematical model of the two pathways and its use in identifying potential effectors of a switching mechanism.

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MS109

A Differential Algebra Method for Finding Identifiable Parameter Combinations of Nonlinear ODE Models

Parameter identifiability analysis for dynamic system ODE models concerns finding which unknown parameters can be quantified from given input-output data. If all the parameters of a model have a finite number of solutions, then the model is said to be identifiable. However, many models are unidentifiable, i.e. the parameters can take on an infinite number of values and yet yield identical input-output data. This problem has been especially apparent in Systems Biology. In this talk, we examine unidentifiable models and a differential algebra method for finding globally identifiable parameter combinations using Groebner Bases. We also discuss computational difficulties in finding these identifiable parameter combinations and explore possible improvements to our algorithm.

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MS109

Disentangling Phylogenetic Mixture Models

Mixture models are used to model the heterogeneity inherent in evolutionary processes. A mixture model is specified by a collection of trees (possibly with repetitions). I will discuss ongoing work on the identifiability of phylogenetic mixture models. The best results in this area require a mix of techniques from algebraic geometry and discrete mathematics.

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MS110

Exploiting Sparsity in Derivative Computation

Jacobian and Hessians matrices that arise in large-scale computations are typically sparse. We discuss combinatorial algorithms and software we have developed for making the computation of such matrices using Automatic Differentiation efficient in terms runtime and memory usage. We illustrate the advantages the methods afford using a numerical optimization problem in chemical engineering as an example.

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MS110

Automating Sparse Gradient Computations in Optimization of Partially Separable Functions

Optimization problems often exhibit *partial separability* (PS). A function f is partially separable if f can be represented in the form $f(x) = \sum_{i=1}^{m} f_i(x)$ where f_i depends on $p_i \ll n$ variables. The sparsity of the Jacobian (and Hessian) of f can be exploited by computing the sparse Jacobians of the elemental functions first. We present PS support in ADIC2 by using the ColPack coloring toolkit and demonstrate it with a TAO optimization example.

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MS110

An Efficient Overloaded Method for Computing Analytic Derivatives of Mathematical Functions in MATLAB

An operator-overloaded method is presented that generates analytic derivatives of mathematical functions defined by MATLAB computer code. The method implements forward more automatic differentiation in a manner that produces a source code that contains the derivative of the original function. Because a new source code is produced, the method can be applied recursively to generate derivatives of any order. A description of the method is given and its effectiveness is demonstrated on three examples.

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MS110

Computing Higher-order Derivatives: Approaches, Tools and Uses

The approximation errors of finite difference schemes for computing higher-order derivatives make their use in practical applications unattractive. Except for cases where analytical derivatives are available, only algorithmic differentiation (AD) can provide derivatives of an arbitrarily high order with machine precision. The talk will cover the basic approaches used in the AD context for computing such derivatives, cover the most relevant AD tool implementations, and the computational complexity. It will briefly highlight current developments addressing heterogeneous computing hardware. The talk will conclude with example uses of higher-order derivatives and practical tool applications from ODE solvers, model reductions, path continuation methods, and others.

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MS111

Weather, Uncertainty, Supercomputing, and Cancer: Research Experiences for Math Majors at Arizona State University

This talk describes innovative programs that involve mathematically talented students at the sophomore through senior level. Interdisciplinary group projects and related courses in modern applications of mathematics, including ensemble forecasting, biomedical models, state estimation, finance, and high-performance computing, are offered to 11 to 16 juniors each year (with beneficial impacts on the graduate program as well). I will also discuss efforts to develop a 21st Century undergraduate mathematics curriculum.

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MS111

Experiences in Running the STAGE Program

'Smooth Transition for Advancement to Graduate Education' (STAGE), is a multi-year NSF-funded eight-week summer research experience for underrepresented minority undergraduate students which intends to immerse the participants, mainly from the HBCUs, in an intensive training program that includes (a) crash courses,(b) guided research, and (c) professional developments. This talk is based on the rewarding experience of managing STAGE in 2011 which can help other researchers in running similar programs nationwide.

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MS111

Excel-lent Experiences: Computational Research Internships

Professors can help undergraduates excel through obtaining meaningful CSE research internships. Such internships can enhance students' professional and personal lives and can add new dimensions to a school's program. With students' inexperience, active involvement by professors is usually a crucial. Using numerous "success stories," this talk explores how advisors can help students obtain and benefit from computational research experiences.

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MS111

Undergraduate CSE Programs in the U.S.

In this talk, a brief survey of some of the different models of undergraduate computational science and engineering programs will be presented. This will highlight some current best practices that can be extended to applied mathematics in general. relevant activities of SIAM's Education Committee will also be presented including possibilities for outreach into the K-12 community.

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MS112

Addressing the Materials Genome Initiative through the AFLOWLIB.ORG Consortium: Thermoelectric Properties of Sintered Compounds with High-throughput Ab-initio Calculations

In this presentation we will describe the aflowlib.org consortium and give some examples of its use including scintillator, thermoelectrics and topological insulators research.

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MS112

Data Mining Applications for Knowledge Discovery in Materials Science: Promises and Challenges

Extensive materials databases are available for new knowledge discovery. However, in spite of considerable advances in data mining techniques, materials scientists still lack practical data mining tools to manage and transform the data into actionable knowledge. We have initiated a series of computational experiments with various materials data in an attempt to create such tools. An overview of promises as well as challenges of such studies will be presented.

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MS112

Informatics for the Materials Genome: a Minimalist Perspective

The recently announced Materials Genome Initiative raises a fundamental question of whether materials can in fact have a "gene". Implied in the term of "genome" is the idea for the need for large quantities of data. This talk ventures to show, however, that we in fact need to seek the minimal amount of data . Applications of statistical inference integrated into a variety of data mining tools for materials design are presented.

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MS112
USPEX: Evolutionary Crystal Structure Prediction as a Tool in Materials Design

The evolutionary methodology USPEX for crystal structure prediction [1] provides, with high reliability and efficiency, the stable and low-energy metastable structures of a given compound at given P-T-conditions. Theory of energy landscapes of solids [2] gives tools that greatly enhance structure prediction. The following results will be discussed: 1. Theoretical and experimental evidence for a new stable high-pressure phase of boron, γ-B [3], showing superhardness and charge transfer between boron. 2. New high-pressure phase, a transparent insulator, was found for sodium [4]. 3. High-pressure phases of group IV hydrides methane CH4 [5], silane SiH4 [6], germane GeH4 [7] and stannane SnH4 [8]. We found much more stable phases of SiH4 and SnH4 than previous random-sampling predictions, and unusual structure of the superconducting phase of GeH4 with high Tc= 64. CH4 decomposes into diamond and hydrogen within interiors of giant planets; this process is important for understanding the energy balance of Neptune. Our method has been extended to enable efficient prediction of the structure of nanoparticles and surface reconstructions, which opens doors for many geochemical applications, as well as predictive studies of nanomaterials and catalysis. References [1] Oganov A.R., Glass C.W., J.Chem.Phys. 124, 244704 (2006) [2] Oganov A.R., Valle M., J.Chem.Phys. 130, 104504 (2009) [3] Oganov A.R., Chen J., Gatti C., et al., Nature 457, 863 (2009) [4] Ma Y., Eremets M.I., Oganov A.R., et al., Nature 458, 182 (2009) [5] Gao G., Oganov A.R., et al., J.Chem.Phys. 133, 144508 (2010). [6] Martinez-Canales M., Oganov A.R., et al., Phys.Rev.Lett. 102, 087005 (2009) [7] Gao G., Oganov A.R., et al., Phys.Rev.Lett. 101, 107002 (2008). [8] Gao G., Oganov A.R., et al. (2010). Proc.Natl.Acad.Sci. 107, 1317 (2010).

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MS113
Efficient Spectral-Galerkin Methods for High-order Equations and Systems of Coupled Elliptic Equations with Applications to Phase-field Models

Abstract not available at time of publication.

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MS113
Computational Issues for Multi-physics, Multi-Phase Equations

Abstract not available at time of publication.

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MS113
Using GPUs to Compute Solutions to the Functionalized Cahn-Hilliard Equation

We present a nonlinear semi-implicit numerical scheme for computing solutions to the evolution equation,

$$u_t = \Delta(\epsilon^2\Delta - W'(u) + \epsilon^2\eta)(\epsilon^2\Delta u - W'(u)), \qquad (4)$$

that describes pore network formation in a functionalized polymer/solvent system as described by the Functionalized Cahn-Hilliard Model. The physical process is defined by multiple time-scales: short time phase separation, long time network growth, and slow evolution to steady state. This requires very long simulations, so our scheme is designed to be unconditionally gradient stable allowing for adaptivity in the time stepping while preserving the discrete energy law. The gradient stability derives from the semi-implicit splitting of the chemical potential into contractive and expansive components. We present a novel iteration for solving the nonlinear equation with a Fourier spectral method, and numerical results are shown with a 10x speedup using Graphics Processing Units (GPUs).

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MS113
Variational Multiscale Models for Biomolecular Systems

A major feature of biological science in the 21st Century will be its transition from a phenomenological and descriptive discipline to a quantitative and predictive one. I will discuss the use of differential geometry theory of surfaces for coupling microscopic and macroscopic scales on an equal footing. Based on the variational principle, we derive the coupled Poisson-Boltzmann, Nernst-Planck (or Kohn-Sham), Laplace-Beltrami and Navier-Stokes equations for the structure, dynamics and transport of ion-channel systems. As a consistency check, our models reproduce appropriate solvation models at equilibrium. Moreover, our model predictions are intensively validated by experimental measurements. Mathematical challenges include the well-posedness and numerical analysis of coupled partial differential equations (PDEs) under physical and biological constraints, lack of maximum-minimum principle, effectiveness of the multiscale approximation, and the modeling of more complex biomolecular phenomena.

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MS114

A Dynamic Model of Polyelectrolyte Gels

Abstract not available at time of publication.

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MS114

Models with Increasing Complexity for Hydrogel/enzyme Feedback Oscillations

Abstract not available at time of publication.

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MS114

Computations of Moving and Deforming Objects in Biological Flows

Abstract not available at time of publication.

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MS115

Noise-induced Transitions of Barotropic Flow over Topography

We study the noise-induced transitions in a climate system modeled by the barotropic quasi-geostropic equations with topography. The stochastic dynamic is constrained on a constant energy surface and it exhibits metastable behavior: The system is likely to stay trapped for a long time near one state until it switches to another. The metastable states are characterized by the strength of the zonal flow. We compute the maximum likely-hood transition paths and the transition rates between the metastable states using the string method. We first study a truncated one-mode ODE model, then generalize the results to the full PDE model. This is a joint work with Xu Yang and Eric Vanden-Eijnden.

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MS115

Analysis of Parallel Replica Dynamics

Parallel replica dynamics was first proposed by A.F. Voter as a numerical tool for accelerating molecular dynamics simulations characterized by a sequence of infrequent, but rapid, transitions from one state to another. An example would be the migration of a defect through a crystal. Parallel replica dynamics accelerates this by simulating many replicas simultaneously, concatenating the simulation time spent of the ensemble, as thought it were a single long trajectory. This leads to several numerical analysis questions: Is parallel replica dynamics doing what we think it is? For what systems will it be useful? How do we implement it efficiently? In this talk, I will thoroughly describe the algorithm and report on progress towards rigorous justification. Open questions will also be highlighted.

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MS115

Escape from An Attractor: Importance Sampling and Rest Point

We discuss asymptotically optimal importance sampling schemes for the estimation of finite time exit probability of small noise diffusions that involve escape from an equilibrium point. The appearance of the rest point complicates the prefactor of the second momentum of the ordinary state-dependent importance sampling estimator. Our analysis points out a useful and efficient scheme to obtain a nice prefactor by using the linear quadratic regulator near the rest point.

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MS116

The Adaptive Finite Element Simulations for the Electronic Structures

Abstract not available at time of publication.

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MS116

Multiscale Modeling and Model Computation for Scanning Near-Field Optical Microscopy

Abstract not available at time of publication.

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MS116

Scattering and Resonances of Thin High Contrast Dielectrics

Abstract not available at time of publication.

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MS116

Some Reconstruction Algorithms in Quantiative Photoacoustic Tomography

In quantitative photoacoustic tomography (qPAT) we aim at reconstructing physical parameters of biological tissues from "measured' data of absorbed radiation inside the tissues. Mathematically, qPAT problems can be regarded as inverse problems related to some elliptic partial differential equations. We present in this talk some new reconstruction strategies for inverse problems in qPAT with different types of available data.

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MS117

Liszt: A Domain Specific Language for Partial Differential Equations

Liszt is a domain specific language to simplify solving partial differential equations (PDE) on parallel computers and graphics processing units (GPU). Liszt is a high level language that contains constructs specific to PDE solvers such as finite-volume or finite-element methods on unstructured grids. Topological objects like mesh, cell, face, edge and vertex are part of the language. Knowledge of the mesh connectivity allows the compiler to automatically reason about data dependency and schedule communication (eg, MPI calls). As a result Liszt code does not contain any explicit parallel instruction, such as inter-node communication, aside from the use of parallel for loops to iterate over mesh objects. A Liszt code is very portable. The source to source compiler can take the same code as input and produce MPI code for clusters, openMP code for multicore processors, and CUDA code for GPUs. The performance of Liszt matches or in some cases exceeds hand tuned code.

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MS117

Linear Solvers at Extreme Scale: Challenges and Opportunities

The emergence of scalable manycore computing systems presents fundamental challenges and opportunities for linear equation solvers. In this talk we discuss the role of processor and memory architecture, system faults and problem size in guiding linear solver algorithms research and development. In particular, we discuss new opportunities for making linear solvers faster, more robust and resilient to system faults.

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MS117

A Heterogenous Scale-bridging Kinetic Solver for Emerging Architectures

The advent of modern parallel architectures, and the promise of exascale computing resources, brings new challenges to computational science. Dependably taking advantage of billion-way parallelism and distinct levels of parallelism will stress solver algorithms. We are developing a broadly applicable scale-bridging solver algorithm to help meet some of this challenge. Development of similar moment-based acceleration methods can be found in a variety of application areas such as neutron transport, thermal radiation (photon) transport, kinetic plasma simulation. We will provide algorithm fundamentals and open research questions. We will provide some indication of algorithm performance on emerging architectures.

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MS117

Co-Design and You

In this talk I will give a high-level, general discussion of the DOE ASCR Exascale Co-Design Centers and the role of applied mathematics in extreme-scale scientific computing.

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PP1

A Gpu Implementation of Von Mises-Fisher Distribution Algorithm for Polymer Conformation Anal-

ysis

The statistical representation of polymer conformations is very important because it is impossible to track all relevant microscopic variables for each polymer in a polymer-laden solution due to the huge number of degrees of freedom. In our study we consider one of the most descriptive kinetic models of polymer, Kramers' bead-rod model, where the probability density function models the angle of each rod with respect to the fixed coordinate axes. Towards this goal we apply von Mises-Fisher distribution for a polymer conformation distribution. The hard and soft assignment methods of clustering of the Expectation-Maximization algorithm are used to cluster the mixture model which have been implemented in parallel using CPU and GPU based platforms. We demonstrate that the GPU-accelerated version of the clustering algorithm is significantly faster than the CPU version.

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PP1

Pollutants Transport Simulation in Atmospheric Boundary Layer Using Stabilized Finite Element Formulations

This work deals with a numerical method based on the Galerkin Least Square scheme for a two-dimensional model of pollutant dispersion in the atmosphere. The model, which is described through a diffusion-convection equation, accounts for pollutant emission from the soil and from an elevated source. It also accounts for diurnal changes in the atmospheric stability conditions via parametric models for turbulent diffusion and wind speed. Numerical results are obtained and compared with results available in the literature.

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PP1

Advanced Optimization Techniques for Entropy-Based Closures in Slab Geometry

Entropy-based moment closures are a parallelizable simulation technique with attractive theoretical properties for reducing the state-space of the kinetic equation, but the defining optimization problem is arbitrarily poorly conditioned for moments of highly anisotropic distributions. We resolve this difficulty by adaptively selecting the polynomial basis defining the moments, and when the optimization problem cannot be solved in finite precision, we find a physically similar solvable problem.

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PP1

Alternate Powers in Serrin's Swirling Vortex Solutions

We consider a modification of the fluid flow model for a swirling vortex developed by J. Serrin, where velocity decreases as the reciprocal of the distance from the vortex axis. Recent studies, based on radar data of selected severe weather events, indicate that the angular momentum in a tornado may not be constant with the radius, and thus suggest a different scaling of the velocity/radial distance dependence. Motivated by this suggestion, we consider Serrin's approach with the assumption that the velocity decreases as the reciprocal of the distance from the vortex axis to the power b with a general $b > 0$. This leads to a boundary-value problem for a system of nonlinear differential equations. We analyze this problem for particular cases, both with nonzero and zero viscosity, discuss the question of existence of solutions, and use numerical techniques to describe those solutions that we cannot obtain analytically.

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PP1

High Order Numerical Method for the Nearly Singular Integration of the Stokes Kernel

Simulating Stokesian particulate flows using integral equations requires the resolution of nearly singular integrals (evaluation of the fluid variables near the surface of a particle), which are inaccurate using standard quadrature rules. We propose a method to resolve this numerical difficulty. We partition the space around a particle into two different zones: we use quadrature in the far zone and we interpolate in the nearly singular zone. We present results in two dimensions.

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PP1

An Axisymmetric Boundary Element Method for Modeling Biphasic Articular Cartilage Mechanics

In comparing the stress, strain, and deformation of healthy and osteoarthritic cartilage under an applied load, differences in parameter values can give insight into the nature and progression of osteoarthritis. An axisymmetric Laplace-domain boundary element method is presented for solving the boundary integral equations modeling the response of biphasic cartilage tissue under mechanical loading, which involve fundamental solutions of the governing PDEs. Simulation of confined compression stress relaxation of a biphasic cartilage cell is shown.

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PP1

Predicting Bifurcations in Dynamical Systems

Nonlinear dynamical systems, which include models of the Earths climate, financial markets and complex ecosystems, often undergo abrupt transitions that lead to radically different behavior. The ability to predict such qualitative and potentially disruptive changes is an important problem with far-reaching implications. For a nonlinear dynamical system with multiple parameters, we combine Conley index theory with machine learning techniques to accurately predict global bifurcations.

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PP1

AWM - Time Asymptotic of Non-Darcy Flows with Total Boundary Flux

We study a time asymptotic of the non-linear Forchheimer flows in porous media with given total flux and constraints on the pres- sure trace on the boundary. We prove that if total flux stabilizes then the difference between pressure average inside domain and on the boundary stabilizes as well. The refined comparison of fully transient and certain time-invariant pressure was performed. These results can be applied in reservoir engineering and other problems modeled by diffusive equations.

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PP1

Faraday Waves on Surfactant-Covered Thin Films

Liquid layers under vertical vibration give rise to a surface wave pattern known as Faraday waves. In this work, the effects of surfactants on Faraday waves are explored under the assumption that the depth of the liquid layer is small. Owing to the importance of inertial effects, the standard lubrication approximation is not suitable and extended thin film type approximation must be used. Numerical simulations and linearized analysis of this modified model are presented.

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PP1

Multi-Frequency Iterative Integral Equations Method for the Shape Reconstruction of An Acoustically Sound-Soft Obstacle in the Presence of Multiple Scatterers

We present a method to solve the problem of obtaining a reconstruction of a planar acoustically sound-soft obstacle from the measured far-field pattern generated by plane waves with a fixed incidence and varying frequencies. We solve iteratively the problem for each frequency, from the lowest to the highest, using as initial guess the solution given by the previous frequency. We present numerical results showing the benefits of our approach.

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PP1

Particle Methods for Geophysical Flows on the Sphere

We develop a fluid dynamics solver for spherical domains with a focus on applications related to the "dynamical cores" of global circulation models. We use a tree-structured Lagrangian grid and intermittent interpolation of the Lagrangian flow map to avoid inaccuracies caused by mesh distortion without introducing significant mass error. Interpolation is carried out using integral convolution with a regularized delta kernel. Fluid equations are solved using Green's function integral solutions for the velocity stream function and potential.

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PP1

Software Development for a Three Dimensional Gravity Inversion and Application to Study of the Border Ranges Fault System, South Central Alaska

Our research involves the testing of several plausible density models of structure along the Border Ranges Fault System in South-Central Alaska by developing a novel, 3D inversion software package. The inversion utilizes gravity data constrained with geophysical, borehole, and surface geological information to produce a density solution. The novel inversion approach involves directly modeling known geology, initially free-air corrected data, and revising "a priori" uncertainties on the geologic model to allow comparisons to alternative interpretations.

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PP1

Numerical Solution of Integral Equations in Solidification and Laser Melting

We consider the evolution of the liquid-solid interface in a freezing or laser-induced melting process. Using the Green's representation theorem for the heat equation and the Stefan condition we obtain a system of nonlinear integro-differential equations in space and time. The integral equations are discretized with the Nyström method which leads to an efficient time stepping scheme to determine the position and velocity of the interface with given material properties.

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PP1

Stochastic Approximated-Gradient Optimization Methods for Oilfield Well Placement

Well placement is critical to optimal hydrocarbon resource management. This work compares the performance of Ensemble-based Optimization (EnOpt) and Fixed-Gain SPSA (FSP) for optimal well placement. These algorithms belong to the broad class of stochastic approximated-gradient methods and offer several practical benefits: They combine the advantages of both gradient-based and stochastic optimization algorithms without the corresponding computation effort, do not require access to simulator code and the gradient approximation is independent of the problem dimensions.

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PP1

Spatio-Temporal Calcium Smoothing in Dendritic Trees

To understand how animals learn it is necessary to study changes in the strength of synaptic connections between neurons. It is thought that synaptic plasticity underlies learning and memory at a cellular level. Therefore the mechanisms of synaptic plasticity have been a key question in neuroscience. However, current imaging techniques are limited in their ability to capture the electric properties of a neuron at the fine scales necessary to address this problem. We use fast, random access, fluorescent multi photon microscopy to indirectly measure calcium concentration from different locations on a cell. The recordings of light intensity of the probe molecules (fluorophore) is spatially sparse and have low signal to noise ratio. Therefore, we propose two methods to infer the underlying calcium signal across the entire dendritic tree from such recordings. The first method is a simple least squares estimate, which recovers the signal at isolated spatial locations, followed by spatial interpolation using splines. The second method uses Bayesian inference to smooth signal. Both algorithms have the ability to infer the underlying calcium signal up to some affine transformation. Each approach has advantages and disadvantages in complexity and computing time. However, we show how the recovered traces from each algorithm can provide insight into the mechanisms that underlie synaptic plasticity

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PP1

AWM - Tumor Growth in Complex, Evolving Geometries: A Diffuse Domain Approach

In this poster, we present a new diffuse domain method for simulating tumor growth in complex, evolving geometries, taking into account homotype adhesion between tumor cells and heterotype adhesion between the cells and the basement membrane. We develop an adaptive energy-stable nonlinear multigrid method to solve the governing equations efficiently. Two and three dimensional simulations are performed. This provides a model for ductal carcinoma in situ.

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PP1

Singular Limits of Geophysical Fluid Dynamics in Spherical and Bounded Domains

We study 2D geophysical fluid models in physically relevant, fast rotating domains. The initial data are unprepared. The first model is the rotating shallow water equations with solid-wall boundary conditions. We prove convergence rates of a singular limit problem as the Rossby number goes to zero. The second model is incompressible Euler equations on a fast rotating sphere. The time-averages of solutions are shown to be approximately longitude-independent zonal flows, which is due to the non-flat geometry.

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PP1

Crossover Design for Studying Obstructive Sleep Apnea

The physiological response to sleep apnea was determined from beat to beat blood pressure in 16 healthy subjects by a series of breath hold maneuvers. The experiments were done for both sitting and supine posture of the subject. For finding the difference in breath hold related physiological changes during different protocols and posture, crossover design is carried out on the area under blood pressure waveform during breath holds and the results will be presented.

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PP1

Modeling and Simulating Flow-Induced Fluctuations in Polymer Solutions

Polymer solutions under flow exhibit anisotropically amplified concentration fluctuations due to stress/concentration coupling. The full model incorporates a two-fluid approach with polymer stress described by the Rolie-Poly equations together with thermal noise, introduced consistently by application of the fluctuation-dissipation theorem. Perturbations of the resulting Langevin equations about homogeneous, in particular extensional, flow are examined. A method of characteristics solver is developed and the predictions are compared with experiments on a polystyrene solution in extensional flow.

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PP1

AWM - Curve Matching Using Discrete Integral Invariants

As a result of its use in medical imaging, aerial photography, and handwriting recognition, curve matching is a significant problem in the field of image analysis. Previous works propose integral invariants as a robust solution for the curve matching problem. However, these invariants rely on a parametric equation fit to the curve and in many real world applications, this fit requires a fair amount of computational work. We generate discrete invariants that require only an ordered set of points. We apply our discrete invariants to the fields of image recognition and object assembly. In this poster, we present examples of curve matching used for handwriting recognition and puzzle completion.

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PP1

A Finite-Element Mmoc Groundwater Model for Gpu's on the Cloud

We use finite-elements with a modified method of characteristics to model a reaction-diffusion problem with advection. Our application of interest is in the area of Groundwater flow with contaminant transport where biofilms are present. The linear system of equations developed from the PDEs governing this physical model are solved on a cluster of GPUs accessed over the Cloud.

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PP1

AWM - Polyhedral Combinatorics For Phylogenetic Trees

Tree agglomeration methods such as Neighbor-Joining and UPGMA continue to play a significant role in phylogenetic research. Polyhedral combinatorics offers a robust toolkit for analyzing the natural subdivision of Euclidean space induced by classifying the input vectors according to tree topologies returned by an agglomerative algorithm. We give a closed form for the extreme rays of UPGMA cones on n taxa via the partition lattice Π_n. We also study the cones induced by the NJ algorithm.

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PP1

Stochastic Heterogeneous Multiscale Modeling of Single Phase Flow in a Porous Media

Risk assessment for carbon sequestration applications requires detailed analysis of multiphase flow through porous media. We present a stochastic Heterogeneous Multiscale Method (HMM) with iterative coupling to model the distributions of macroscopic pressure based upon statistical-based random pore-throat size probability density. We analyzed its impact in a one dimensional macroscopic model, coupled to a two dimensional microscale network model. We further propose a domain decomposition strategy with a highly efficient implementation for large scale simulations.

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PP1

Probabilistic Divide-and-Conquer: a New Method for Exact Sampling with Integer Partitions as an Example

For us, the random objects S whose simulation might benefit from a divide-and-conquer approach are those that can be described as $S = (A, B)$, where there is some ability to simulate A and B separately. Specifically, we require that $A \in \mathcal{A}$, $B \in \mathcal{B}$, and that there is a function $h : \mathcal{A} \times \mathcal{B} \to \{\prime, \infty\}$, so that for $a \in \mathcal{A}$, $\lfloor \in \mathcal{B}$, $h(a, b)$ is the indicator that "a and b fit together to form an acceptable s.' Furthermore, we require that A and B be independent, and that the desired S be equal in distribution to $(\ (A, B)|h(A, B) = 1)$. This description, independent objects conditional on some event, may seem restrictive, but very broad classes — combinatorial assemblies, multisets, and selections — fit into this setup.

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PP1

Numerical Methods for Delay Differential Equations with Applications to Biology

In this poster we present a numerical method for delay differential equations with application to some biology problems. Two different applications are presented. The first one is R.V Culshaw and S. Ruan s DDE model of cell-free viral spread of human immunodeficiency virus (HIV) in a well-mixed compartment such as the bloodstream. A discrete time delay was introduced to describe take into account the time between infection of a CD4+ T-cell and the emission of viral particles at the cellular level. We present an analytic stability analysis of the endemically infected equilibrium. we then present a numerical analysis of the stability and bifurcation process of the same equilibrium using numerical tools. The second application is the DDE model proposed by Barlett and Wangersky. Their model is a Non-Kolmogorov-Type predator prey model with two discrete times delay. We again present an analytic and a numerical analysis of the stability and bifurcation process of the steady state solutions. Numerical simulations are presented to illustrate the results.

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PP1

A Predictive Model for Geographic Statistical Data

Any planar map may be transformed into a graph. If we consider each country to be represented by a vertex (or node), if they are adjacent they will be joined by an edge. To consider how trends migrate across boundaries, we obtain relevant measures of the statistic we want to consider; namely, the index of prevalence, and the index of incidence. We define a cycle by a given unit of time, usually a year. We then propose various alternate equations whereby, by parametrizing various variables, such as population size, birth rate, death rate, and rate of immigration/emigration, we calculate a new index of prevalence/index of incidence, for the next cycle. For a given data set, each statistic we consider may propagate by a different equation, and/or a different set of parameters; this will be determined empirically. What we are proposing is, technically, to model how a discrete stochastic process propagates geographically, according to geographical proximity. Very often, statistics that depend on geographical proximity are tabulated by variables that are not; i.e., alphabetically. Such a predictive model would be relevant in areas such as public health; and/or crime mapping, for law enforcement purposes. We present an application using a GIS (geographic information system).

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PP1

Investigations of Cai's Power Law for Strong Tornados

We investigate the consequences of power laws and self similarity in mesocyclones and tornados as presented in the work of H. Cai. We give a model for tornado genesis and maintenance using the 3-dimensional vortex gas theory of Chorin. High energy vortices with negative temperature in the sense of Onsager play an important role in the model.

We speculate that the high temperature vortices formation is related to the helicity they inherit as they form or tilt into the vertical. We also exploit the notion of self similarity to give justification for power laws corresponding to weak and strong tornados given by Cai. Doing a nested grid simulation using ARPS we find results consistent with Cai's scaling.

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PP1

Convergence in Mallows-Wasserstein Distance of Randomly Indexed Partial Sums and Upper Bounds for the Ruin Probabilities

Abstract: Classical risk processes are modelled with a Poisson arrival process along with light-tailed claim variables. However, some real data measurements may not be compatible with the assumption of the finiteness of the second moment. In this case, heavy-tailed rewards may arise as a suitable approach. By considering a heavy-tailed renewal reward dependent process and by making use of the Mallows-Wasserstein distance, we study the asymptotic properties of the resulting randomly indexed partial sums and obtain upper bounds for ruin probabilities. Applications to data traffic in cumulative broadband networks as well as buffer overflow probabilities are also presented.

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PP1

Statistical Methods for Detecting Fraudulent Prescriptions

In the medical field, fraud, waste, and abuse are prevalent. A large percentage of medical expenditures are for procedures later deemed unnecessary. In order to cut down this rate, this project focuses on detecting unneeded prescriptions by comparing insurance claims against normal behavior patterns. The prescriptions are sorted by similar medical claims and analyzed within these groups. Abnormal transactions are then detected and flagged for human review.

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PP1

Unsupervised Methods to Detect Health Care Waste

Detecting fraud is a big part of credit card management. We are trying to apply similar methods to detect waste in health care. A good portion of health care procedures and drugs are unnecessary. We use data that contain health insurance claims to attempt to detect the unnecessary procedures and drugs. It isnt explicitly obvious from the data which claims are wasteful, so we must use unsupervised methods. These methods include developing a measurement of similarity between different procedures.

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PP1

Three-Dimensional High-Resolution Simulation of Convective Mixing

Dissolution by convective mixing is an essential trapping mechanism during CO2 sequestration. The injected CO2 mixes with brine and creates mixture denser than both initial fluids, leading to a Rayleigh-Benard type instability, which greatly accelerates the dissolution process.While 2D analyses on this phenomenon have elucidated various aspects of this mechanism, full 3D studies are scarce. We present high-resolution, 3D simulations of convective dissolution, and discuss the validity of quantitative results derived from lower-dimensional models.

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PP1

Fast Algorithms for Inverse Problems of Reaction-Diffusion-Advection Equations

We present a method for the solution of an inverse problem with parabolic PDE constraints. The constraint is a reaction-diffusion-advection equation. We discuss two numerical methods to solve the associated least squares inverse problem, one based on a direct solve and one based on a randomized SVD. Numerical tests are performed to show the effectiveness of the methods for different cases, that is to compare the speed of calculations and the accuracy of the predicted data.

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PP1

A Fast Algorithm to Solve Slow Incompressible Steady Flows

We present a high order fast algorithm to solve the boundary value problems associated with the inhomogeneous Bi-

harmonic equation in the interior of a unit disk of the complex plane using uniform and non-uniform grid. The fast algorithm is based on the representation of the solution in terms of Green functions, uniform and non-uniform fast Fourier transforms and some recursive relation derived in the Fourier space. Performance of this algorithm on non-uniform mesh and with singular source terms are some of the attractive features of this algorithms. This algorithm has been implemented, validated and applied to solve several interesting applied problems from fluid mechanics and electrostatics.

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PP1

Analysis of Interfaces for the Nonlinear Diffusion-Convection Equations

The problem of determining the short-time behavior for interfaces of nonlinear diffusion equations, known as a Barenblatt problem, was first formulated in the 1950s. A full solution of the Barenblatt problem for the related problem of reaction-diffusion was given in 2000 [Abdulla and King, SIAM J. Math. Anal.] but the problem remains open for the diffusion-convection case. In this work we first identify the regions in the parameter space relevant for the expanding, shrinking and stationary interfaces. We fully characterize the case when diffusion dominates over the convection. We prove explicit asymptotic formulae for the expanding interface and local solution. The methods used are maximum principle for the weak solutions, comparison theorems and scaling techniques. We also analyze self-similar solutions and travelling waves in the borderline case.

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PP1

Identifying Fraud with Bayesian Networks

Detecting fraud, waste, and abuse in healthcare is an important topic. Our approach aims to identify anomalies in medical insurance claims data by combining a prior fraud likelihood rating with Bayesian network classification. We calculate the probability of an insurance claim with the help of a Bayesian network and compare this probability with the probabilities of other claims. By assuming that most insurance claims are legitimate, we can use this comparison to tag low probability claims for further investigation.

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PP1

Minimizing Rational Functions by Exact Jacobian SDP Relaxation Applicable to Finite Real Singularities

This paper consider the minimization of rational functions with or without polynomial constraints. We reformulate this problem as polynomial optimization by homogenization. We give some conditions under each of which we show the equivalence of these two optimizations. As a special case, these two optimizations are always equivalent when there are no constraints. We also investigate the relations between the achievabilities of their optima. The exact Jacobian SDP relaxation proposed by Jiawang Nie is employed to solve the polynomial optimization obtained by homogenization. We also prove that the assumption of the smoothness in Nie's paper under which the Jacobian SDP relaxation is exact can be weakened as the finiteness of real singularities. Some numerical examples are given in the end to illustrate the efficiency of our method.

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PP1

Statistics of Solar Cycle-La Nina Connection: Correlation of Two Autocorrelated Time Series.

Both the 11-year solar cycle and the El Nino-Southern Oscillation (ENSO) phenomena are quasi-periodic, with periods of 9-11 years and 3-4 years, respectively. There have been claims that the two are correlated, with the Sun at its peak in Sunspot number presumably forcing a cold event in the equatorial Pacific. However both phenomena are also highly auto-correlated. Caution should be exercised when testing for statistical significance of the correlation of two autocorrelated time series. Even if the two time series are independent, the solar peak years can coincide with cold-ENSO by chance, and then persist for many cycles due to their autocorrelation, before drifting apart. We demonstrate that this is indeed the case using the Quinn El Nino Index going back to 1525, which is a chronicle of observation of El Nino related events, and Sunspot Number (SSN) series, which goes back to 1750. Appropriate statistical tests are suggested that can test for correlation taking into account autocorrelation and are applicable to the shorter instrumental records. There is so far no solar peak-La Nina connection found that is statistically significant at 95% confidence level.

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PP1

Topic Analysis and Grouping of Insurance Claims

Latent Semantic Analysis and Latent Dirichlet Allocation are fairly new tools for document and topic analysis. With some simple modifications, these tools can be used for grouping clusters of medical insurance claims to get some interesting results. This process of grouping claims is also helpful in building models for disease progression. Our goal with these tools is to better predict future medical costs given a patient's claim history.

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PP1

Computation and Analysis of Evolutionary Game Dynamics

Biological species (viruses, bacteria, parasites, insects, plants, or animals) replicate, mutate, compete, adapt, and evolve. In evolutionary game theory, such a process is modeled as a so-called evolutionary game. We describe the Nash equilibrium problem for an evolutionary game and discuss its computational complexity. We discuss the necessary and sufficient conditions for the equilibrium states, and derive the methods for the computation of the optimal strategies, including a specialized Snow-Shapley algorithm, a specialized Lemke-Howson algorithm, and an algorithm based on the solution of a complementarity problem on a simplex. Computational results are presented. Theoretical difficulties and computational challenges are highlighted.

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PP1

Explicit Update Scheme for Inverse Elliptic Problems

We introduce an efficient method to recover piecewise constant coefficients occurring in elliptic PDEs as well as the interface where these coefficients have jump discontinuities. We use an output least squares approach with level set and augmented Lagrangian methods. Our formulation incorporates the inherent nature of the piecewise constant coefficients, which allows us to obtain an explicit update formula for them. Numerical examples of Poisson's equation and linear elasticity are given.

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PP1

AWM - Inferring Gang Affiliation for Violent Events with Incomplete Data

Data sets are often plagued with portions of incomplete data. In this case, the data are assumed to be associated with one of N self-exciting point processes that lie on a network. The time and geographical location for all events are known, however the process affiliation is not known for some events. This work proposes an iterative method with a directly calculable score function assigning weights for process affiliation and approximating the process parameters.

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PP1

A Bayesian Approach to Uncertainty Quantification for Stochastic Epidemic Models

We present a method to quantify the uncertainty in predictions made by stochastic models of epidemics. For these types of simulations random events cause important factors, such as epidemic size and duration, to vary over a wide range of values. This makes it difficult for policy makers to base decisions on these types of epidemic models. In this research we use Bayesian techniques to construct distributions for important epidemic quantities from sample runs of the simulation. Once a distribution is found for an output quantity of interest the quality of the model's predictions can be evaluated. We propose a measure to quantify the effectiveness of a stochastic epidemic models predictive ability using these distributions.

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PP1

A Family of Euler-Maclaurin Formulae for N-Point Gaussian Quadrature

The Euler-Maclaurin Formula is a powerful and well-known result from classical numerical analysis relating discrete sums to integrals. One way to establish this equation is by utilizing periodic Bernoulli Polynomials, which can be derived using a generating function, and performing a straight-forward integration by parts. The obtained formula relates the standard trapezoid rule (or the zero-point Gauss Method) of numerical integration to a series of terms involving the Bernoulli Numbers, the derivatives of the function at the endpoints and an error term. My aim in this presentation is to show one can derive an analogous formula based on the midpoint (1-point Gauss Method), 2-point Gauss method, and, in turn, a general family of Euler-Maclaurin formulae for N-Point Gaussian-Legendre Quadrature.

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PP1

A Slow Pushed Front in a Lotka-Volterra Competition Model

We study invasion speeds in the Lotka-Volterra competition model when the rate of diffusion of one species is small. Our main result is the construction of the selected front and a rigorous asymptotic approximation of its propagation speed, valid to second order. From a perspective of linear versus nonlinear speed selection, this front provides an interesting example as the propagation speed is slower than the linear spreading speed. However, our front shares many characteristics with pushed fronts that arise when the influence of nonlinearity leads to faster than linear speeds of propagation. We show that this is a result of the linear spreading speed arising as a simple pole of the resolvent instead of as a branch pole. Using the pointwise Green's function, we show that this pole poses no a priori obstacle to marginal stability of the nonlinear traveling front, thus explaining how nonlinear systems can exhibit slower spreading that their linearization in a robust fashion.

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PP1

Convergence of a Gauss Pseudospectral Method for Optimal Control

A convergence theory is established for approximations of continuous-time optimal control problems using a Gauss pseudospectral method. Specifically, it is shown that, under assumptions of coercivity and smoothness, the Gauss pseudospectral method has a local minimizer that converges in the sup-norm to a local minimizer of the continuous-time optimal control problem. The convergence theory is summarized and examples are provided that agree with the theoretical results.

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PP1

A Fast Spectral Algorithm for the Quantum Boltzmann Collision Operator

Numerically solving the quantum Boltzmann equation (Nordheim-Uehling-Uhlenbeck equation) is challenging due to the multidimensional structure of the collision integral. Comparing to its classical counterpart, the main difficulty comes from the cubic interaction term. We propose a fast spectral algorithm based on a special decomposition of the collision kernel. Numerical results in 2-D and 3-D for both the Bose gas and the Fermi gas are presented to illustrate the accuracy and efficiency of the method.

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PP1

AWM Variance Reduction for Monte Carlo Simulation for European Call Options Under the Coupled Additive-Multiplicative Noise Model

We propose a variance reduction method for Monte Carlo computation of option prices in the context of the Coupled Additive-Multiplicative Noise model. Four different schemes are applied for the simulation. The methods select control variates which are martingales in order to reduce the variance of unbiased option price estimators. Numerical results for European call options are presented to illustrate the effectiveness and robustness of this martingale control variate method.

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PP1

Device Modeling for Organic Solar Cells

Organic solar cells (OSCs) have great potential to play an important role in addressing our future energy needs. A drift-diffusion model is developed to describe the dynamics of excitons and free charge carriers in OSC. Our model predicts the performance of OSC devices by calculating their quantum efficiency and current-voltage curves, as well as many other important physical quantities, such as electric field, and the carrier concentration.

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PP1

Shortest Path for High-Dimensional Data Representation

We show that the power-weighted shortest path length through random points reflects metric deformation affected by the probability density function. Such metric deformations adapt the data structure of the random sample for machine learning purposes. We reason how the power-weighted shortest path length achieves asymptotic consistency in data clustering and connects to classical single-linkage clustering. Furthermore, the deformation metric framework will be proposed to encompass and connect spectral methods and shortest paths.

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PP1

Analysis of Optimal Mortgage Termination Under the Cox-Ingersoll-Ross Model

We consider mortgage contracts where the borrower has the option to pay the outstanding balance at any time. In theory, the decision to terminate depends on the yield curve. Assuming the Cox-Ingersoll-Ross model for interest rates, the problem can be formulated as a variational inequality or an equivalent free boundary problem. Existence and uniqueness of a solution as well as regularity of the free boundary will be presented.

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PP1

Computing Characteristic Classes in Algebraic Geometry

Characteristic classes, i.e., Chern and Segre classes of varieties are important invariants in algebraic geometry. We present a method to compute them which works either symbolically using Gröbner bases or numerically using homotopy continuation methods for polynomial equation systems. It has been implemented using Macaulay2 and Bertini.

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PP1

Minimizing Communication in Sparse Matrix-Vector Multiplication Using a Novel Representation

We consider the problem of multiplying a sparse matrix $A \in R^{n\times n}$ with a dense matrix $X \in R^{n\times \ell}$ with the aim of increasing register reuse. A new block compressed format that is shown to have less loads compared with compressed sparse row and block compressed sparse row formats, is proposed. The format stores blocks as bitmaps and is less sensitive to the non–zero structure (in comparison with blocked formats). A C++ based algorithm that decodes blocks in $\mathcal{O}(\backslash\ddagger_{\lfloor})$ time, where nz_b is the number of non–zeros in a block, is developed. Performance comparisons with Intel MKL sparse BLAS and with standard CSR and BSR implementations are presented.

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PP1

AWM - A Stochastic Delay Model for Pricing

In the business world, in addition to equity, corporate bonds are also a main source of funds for many companies. However, depending on the ability of the managers or other reason, it can happen that a company faces bankruptcy. When a company becomes insolvent, the stock value decreases to zero and the equity-holders lose their investments. Naturally, debt-holders would like to make sure that their investments are secured. In order to support companies in this situation and encourage new investments, some government agencies provide loan guarantees. In this presentation, we give a formula for the price of an option used for the pricing of corporate defaultable bonds satisfying a stochastic delay differential equation (SDDE). Assuming that the company value satisfies a SDDE as above, we evaluate government loan guarantees for companies in financial distress.

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PP1

Deforming Cylindrical Hypersurfaces in Hyperbolic Space by Their Harmonic Mean Curvature

We show that under harmonic mean curvature flow cylindrically symmetric hypersurfaces about a closed geodesic in hyperbolic space contract to the geodesic and the shape of the evolving hypersurface becomes like a round cylinder. A novel approach is developed to distinguish the radial and angular principal curvatures of the evolving hypersurface by their qualitative behavior using parabolic maximum principle. The evolution equation is a fully nonlinear degenerate parabolic PDE.

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PP1

Deforming Cylindrical Hypersurfaces in Hyperbolic Space by their Harmonic Mean Curvature

We show that under harmonic mean curvature flow rotationally symmetric hypersurfaces about a closed geodesic in hyperbolic space contract to the geodesic and the shape of the evolving hypersurface becomes like a round cylinder. A novel approach is developed to distinguish the radial and angular principal curvatures of the evolving hypersurface by their qualitative behavior using parabolic maximum principle. The evolution equation is a fully nonlinear parabolic PDE.

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PP1

Mechanism of Default Contagion with Graph Representations

We consider a mechanism of contagion of default following default of Greek banks, in which creditor banks in European countries give proportional haircuts to their creditors, in a sequence of stages. Net liabilities are represented by simple weighted directed graphs and bilateral liabilities by multigraphs. We compare with current data. This includes work by undergraduate student Shuangshi Han, with faculty sponsor Katherine Kime.

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PP1

A Delay-Differential Equation Approach to Determine Insulin Sensitivity

After initial research by Bergman et al. (1985) using mathematical models to determine insulin sensitivity in diabetics, the insulin sensitivity question has largely been ignored in preference of directly modeling the glucose/insulin dynamics in the human body. These models have greatly increased in their complexity and ability to explain clinically observed data. This research aims to reopen the insulin sensitivity question using the more sophisticated techniques that have recently been applied to this field.

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PP1

Linear Response Closure Approximation for Multiscale Systems

Many physical processes involve multiscale dynamics, characterized by time and space scale separation with a large set of rapidly evolving variables and a smaller set of slowly evolving variables. We present a method to obtain a closed system for the slow variables, requiring only a simple calculation of statistics of the fast variables and use of the fluctuation-dissipation theorem. We apply this method to a two-scale model with linear coupling.

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PP1

Accuracy-Enhancing Moving Grid Method for Stratified Flow Calculations

We present the moving grid method an r-adaptive discretization of the underlying system of PDEs. This grid adaptivity allows to dynamically increase resolution in the areas of interest (an interface or a rapid flow variation) while keeping the size of computational mesh unchanged. The method was tested on several stratified flow configurations with sharp density discontinuities and consistently outperformed its static-grid counterpart. Scalability and parallel performance of our solver on a supercomputer will be discussed.

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PP1

Reduced Order Modeling for Dynamic Earthquake Simulations

Motivated by the devastating earthquake and tsunami last year in Japan, we explore the use of reduced order models for subduction zone, megathrust earthquake simulations. The technique we employ uses a few parallel, full physics simulations to build a surrogate model which can be sampled to explore the parameter space. The quantities of interest are the total slip on the fault, slip at the trench axis (where the fault meets the seafloor), and seafloor deformation.

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PP1

A POD Study for a Coupled Burgers Equation

We study the coupled Burgers Equation that share similarities with the Boussinesq equations that are commonly used in thermal-fluid dynamics. A training set" of FE solutions is generated and a POD model reduction scheme is applied. However, the actual dynamics of the system can vary from the dynamics that are contained in the training set. Hence, we investigate the dependence of the reduced order model on the input parameters(especially the Reynolds number).

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PP1

Approximating the Singularities of a Function by Means of Its Fourier-Jacobi Coefficients: An Enhanced Power Method

We modify the method suggested earlier by us and overcome its main deficiency. The method enables the approximation of the locations of jump discontinuities of a function, one by one, by means of ratios of so called higher order Fourier-Jacobi coefficients of the function. It is shown that the location of singularity of a piecewise constant function with one discontinuity is recovered exactly and the locations of singularities of a piecewise constant function with multiple discontinuities are recovered with exponential accuracy. Unlike the previous one, the modified method is robust, since its success is independent of whether or not a location of the discontinuity coincides with a root of a Jacobi polynomial. In addition, some numerical examples are presented.

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PP1

Computational Docking of Molecular Wires to the Reaction Center of Rhodobacter Sphaeroides

Given the worldwide interest in renewable energy, scientists have been exploring the possibility of using bacterial photosynthetic reaction centers to build a new generation of highly efficient photovoltaic devices. To build such devices, molecular wires (MWs) that serve as good conductors to transport electrons from and to the reaction centers are needed. The MWs must dock at specific binding sites within the reaction centers. We explore computational models of docking MWs to the reaction centers.

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PP1

Mixed Methods of Viscoelastic Wave Propagation

We present new mixed finite element methods for wave propagation in viscoelastic solids. We use recently developed mixed finite elements for elasticity with weak symmetry of stress for which we have proved optimal a priori error estimates. We present numerical results which support our error analysis and demonstrate the performance of the methods on problems of practical interest.

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PP1

Vector-Valued Parametric Kernel-Based Interpolation for Two-Dimensional Facial Animations

This paper explores a scattered-data, interpolation-based approach, which uses a vector-valued parametric interpolation method for creating tween frames. Using the blendshapes method, a 27-frame, two-dimensional, facial animation was generated. Key-frames 1, 3, and 27 were then used to produce similar animations with the following interpolation methods: Gaussian RBF,Inverse multiquadratic, C^2 Mate rn, Multiquadratic, and the Distance Function. All methods were then compared and performance adjustments made.

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PP1

A Neuronal Network Model of Drosophila Antennal Lobe

We construct a conductance based neuronal network model of the *Drosophila* antennal lobe with the aim of proposing possible interactions within the antennal lobe that account for the variety of projection neuron activity observed in experimental data. Computational studies using olfactory receptor neuron inputs that mimic experimental recordings demonstrate the possible roles of excitatory local neurons in spreading excitation among glomeruli and in recruiting inhibition.

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PP1

SmartGrid Pricing and Consumer Privacy Constraints

The widespread adoption of SmartGrid technologies promises to radically change the way electricity is delivered and priced, in part by enabling the collection of fine-grained data on customer power consumption. Unfortunately, this usage data can be linked by adversaries to other behaviors, seriously threatening consumer privacy. We explore schemes for maintaining privacy, investigate tradeoffs between privacy and fairness, and model the game that arises between providers and strategic, privacy-conscious electricity consumers.

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PP1

Massively Parallel Adaptive Fast Multipole Method for Volume Potentials

FMM is traditionally used to solve N-body problems with point sources. Here, we present a FMM based solver for volume potentials in 3D, using piecewise polynomials and adaptive octree to represent source distribution and output potential. We use OpenMP and MPI for shared and distributed memory parallelism, and BLAS, FFTW and SSE optimizations are used to get high FLOP rates. We present convergence results for various kernels and show scalability to over 100,000 processor cores.

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PP1

A Network-Patch Model for the Transmission and Emergence of Mosquito-Borne Pathogens

We derive a network-patch model for the spread of mosquito-borne diseases that couples to agent-based spatial epidemic models. The new model accounts for environmental factors, such as rainfall and temperature, and for variations in mosquito-related parameters, including the emergence rates and incubation period of the pathogen. It considers spatial heterogeneity in vector populations without modeling individual mosquitoes, thus reducing computational expense while maintaining accuracy. Our simulations quantify the importance of heterogeneity in predicting the spread of vector-borne diseases.

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PP1

High-Order Nodal Formulation of the Mimetic Finite Difference Method for Elliptic Problems

The high-order nodal formulation of the Mimetic Finite Difference Method for two-dimensional elliptic problems is based on a consistency condition that reproduces exactly the integration by parts formula for polynomials of degree higher than one. This formulation requires different kinds of degrees of freedom, like *moments* of polynomials or normal derivatives at edges. Optimal convergence rate is proved in a mesh-dependent H^1 norm for meshes with very general shaped elements and experimental results confirm this behavior. This presentation is based on joint works with L. Beirao da Veiga and K. Lipnikov.

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PP1

Meshfree Quadratures for Planar Regions

Radial Basis Function (RBF) methods have gained significant attention in the last decade as robust and highly accurate alternatives to classical polynomial methods for function approximation. Here, we present a novel quadrature scheme to approximate integrals in smooth planar regions using RBFs. Preliminary numerical results show the scheme to be spectrally (exponentially) convergent and robust with respect to node location.

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PP1

Numerical Modeling of Flow Over Flexible Vegetation

Understanding the interaction of currents, waves, and storm surge with coastal vegetation is important for coastal and environmental engineering. The existence of vegetation greatly affects flow resistance, but modeling vegetation at small scales is challenging. In particular, plant flexibility is often an important factor in the resistance characteristics. We numerically model the interaction of complex flow fields with flexible vegetation, utilizing the immersed boundary method and stabilized finite element methods on highly-resolved computational meshes.

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PP1

Systems of Conservation Laws for Thermodynamically Consistent Adsorption with Subscale Diffu-

sion

Multicomponent adsorption is typically described by a system of conservation laws in which the nonlinear flux terms come from explicit functional relationships called isotherms. Unfortunately the most popular extended Langmuir isotherm is thermodynamically inconsistent. We discuss analysis and numerical approximation of multicomponent adsorption system where the thermodynamically consistent isotherms are given only implicitly. Additionally, we consider subscale diffusion coupled to the transport and the associated nonlocal in time effects which smooth out the solutions.

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PP1

Multiscale Seismic Imaging

Imaging the Earth's interior requires estimation of mechanical parameters (velocities and densities) that describe a region of the subsurface. Numerical solution of the wave equation involves discretization and a choice of a particular scale of interest. The Earth contains interesting features at many scales (from the millimeter to the kilometer scale). We describe an algorithm for solving the wave equation in which sub-wavelength heterogeneities are captured and incorporated into the macro-scale solution.

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PP1

Pandemic Influenza:Best Strategies to Minimize Transmission Despite Parameter Uncertainty

When under the threat of Pandemic Influenza countries decide to take certain measures in order to contain the transmission of the virus. Given that the parameters of the transmission might not be accurate, the scenarios might be far from reality. We employed the robust optimization framework to determine the most efficient strategies that mitigate the adverse effects of Pandemic Influenza.

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PP1

The Case for Exponential Time Differencing for Neuronal Network Simulations

Exponential time differencing (ETD) has been used for Hodgkin-Huxley-like ODEs by several authors, and is the default integrator in the popular neuronal simulation package GENESIS. We show that the effectiveness of ETD for Hodgkin-Huxley-like ODEs comes from the fact that it prevents overshoot during the very fast rising phase of the action potential, allowing simulations that sacrifice accurate resolution of action potentials without significant loss of overall accuracy. We also propose a second-order ETD scheme.

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PP1

Highly Accurate 3D Nearly Singular Integration

Boundary integral methods often give rise to nearly singular integrals in which the integrand is very steep at a point. Standard integration techniques on such integrals suffer from low accuracy. We develop a highly accurate method for 3D surface integrals with near singularities. The method involves isolation and smoothing of the near singularity with two changes of variables. Stokes flow is used as a test case.

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PP1

Application of Fractional Calculus to Domain Wall Motion

The equation of motion carrying the domain wall motion inside a ferromagnetic material has been solved fractionally using Laplace transform technique for a fractional derivative of the damping term. The solution reduces to the well known result of the simple harmonic oscillator when alpha =0 and to the damping result when alpha =1 where the damping term is proportional to the viscosity of the suspension. Results for different values of alpha and damping ratio are drawn and discussed under special initial conditions.

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PP1

Applying Stochasticity to Models of Rotavirus Disease and Vaccination

Despite significant advances in water quality and hygiene around the world, rotavirus diarhhea continues to be the main cause of severe gastroenteritis across the globe. A two-strain continuous-time Markov chain model of rotavirus infection is formulated. This model considers natural immunity from subsequent infections and the effects of vaccination are analyzed. Although, the disease can not be completely eradicated without perfect vaccination, different scenarios for the reduction of morbidity and mortality are evaluated and compared.

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PP1

Cost Benefit Analysis of Vector Control Strategies for Dengue in Bangkok

We use the data from Queen Sirkit National Institute of

Child Health (QSNICH) from 1973-1999 to estimate the true prevalence of Dengue disease in Bangkok, Thailand using Monte Carlo Markov Chain Simulations. We present preliminary results of a cost benefit analysis on three vector control strategies: Larvicide and Adult control, Blocking transmission and Reducing mosquito biting.

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PP1
The Behaviour of a Thin Ridge Or Rivulet of Fluid

Two problems involving a thin ridge or rivulet of fluid are discussed. Firstly, a ridge on an inclined planar substrate subject to an external airflow directed tangentially to the substrate is considered; in particular, the effect of increasing the strength of the airflow is analysed. Secondly, the gravity-driven draining of a rivulet of fixed width around a large horizontal cylinder is considered; qualitatively different behaviour is exhibited depending on whether the rivulet is "narrow' or "wide.'

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PP1
Use of the String Method to Find Minimal Energy Paths of Droplets on Superhydrophobic Surfaces

Interest in superhydrophobic surfaces has increased due to a number of interesting advances in science and engineering. Here we use a diffuse interface model for droplets on topographically and chemically patterned surfaces in the regime where gravity is negligible. We then apply the constrained string method to examine the transition of droplets between different metastable/stable states. The string method finds the minimal energy paths (MEPs) which correspond to the most probable transition pathways between the metastable/stable states in the configuration space. In the case of a hydrophobic surface with posts of variable height and separation, we determine the MEP corresponding to the transition between the Cassie-Baxter and Wenzel states. Additionally, we realize critical droplet morphologies along the MEP associated with saddle points of the free-energy potential and the energy barrier of the free energy. We analyze and compare the MEPs and free-energy barriers for a variety of surface geometries, droplets sizes, and static contact angles ranging from partial wetting to complete wetting. We also introduce an unbiased double well potential in the diffuse interace model by introducing a chemical potential that is fixed for a given simulation. We find that the energy barrier shifts toward the Wenzel state along the MEP as the height of the pillars increases in the topographically patterned case while a shorter energy barrier exists and is more centered along the MEP for pillars of shorter height. More importantly, we demonstrate the string method as a useful tool in the study of droplets on superhydrophobic surfaces by presenting a numerical study that finds MEPs in configuration space, critical droplet morphologies and free-energy barriers which in turn give us a greater understanding of the free-energy landscape.

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PP1
Exact Chirped Soliton Solutions for 1D Gross-Pitaevskii Equation with Time-Dependent Parameters

The Gross-Pitaevskii equation describing the dynamics of a Bose-Einstein condensates at absolute zero temperature, is a generalized form of the Nonlinear Schroedinger equation. In this work, the exact one bright soliton solution of 1D GP equation with time-dependent parameters is directly obtained by using the well known Hirota method under the same conditions as Ref (10). In addition the two-soliton solution is also constructed effectively.

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PP1
Small Steady Self-Similar Inviscid Flow

We consider solutions of the 2-d compressible Euler equations that are steady and self-similar. Examples arise naturally at interaction points in genuinely multi-dimensional flow, and we are able to classify all possible solutions that are L^∞-close to a constant supersonic background. As a special case we prove that solutions of 1-d Riemann problems are unique in the class of small L^∞ functions, and more generally that all solutions are necessarily BV.

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PP1
Computing An Approximation to the Helmholtz Equation with a High Contrast Thin Scatterer Present

In this poster, we present new computations stemming from the work of Moskow, Santosa, and Zhang [S. Moskow, F. Santosa, J. Zhang. *An Approximate Method for Scattering by Thin Structures.* SIAM J. Appl. Math. 66, pp. 187-205]. We compute solutions to the Helmholtz equation with a high contrast thin scatterer present where the diaelectic constant is discontinuous. We then compare the accuracy of a leading term approximation under such conditions.

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PP1

Snakes and Ladders: Stability of Fronts and Pulses

The subject of this poster are localized patches composed of spatially periodic structures. These patterns often exhibit snaking: in parameter space, the localized states lie on a vertical sine-shaped bifurcation curve so that the width of the underlying periodic pattern increases as one moves up along the bifurcation curve. The issue addressed here is the stability of these structures as a function of the bifurcation parameter.

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PP1

AWM Physiologically-Based Pharmacokinetic (pbpk) Modeling of Metabolic Pathways of Bromochloromethane in Rats.

An updated PBPK model for bromochloromethane is generated and applied to two different metabolic hypotheses: 1) a two-pathway model using CYP2E1 and glutathione transferase enzymes, and 2) a two-binding site model where metabolism occurs only with CYP2E1. Our computer simulations show that both hypotheses describe the experimental data in a similar manner. In addition, we explore the sensitivity of different parameters for each model using our obtained optimized values and explore their applications to risk assessment.

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PP1

On the Spectral Stability of Soltion Solutions of the Vector Nonlinear Schrödinger Equation

We consider a system of coupled cubic nonlinear Schrödinger (NLS) equations

$$i\frac{\partial \psi_j}{\partial t} = -\frac{\partial^2 \psi_j}{\partial x^2} + \sum_{k=1}^{n} \alpha_{jk}|\psi_k|^2\psi_j \qquad j = 1, 2, \ldots, n$$

where $\alpha_{jk} = \alpha_{kj}$ are real. The stability of solitary wave solutions is examined numerically using Hill's method (Deconinck, B. and J. N. Kutz. J. Comput. Phys., 219: 296-321, 2006). Our results extend the analysis of Nguyen (Commun. Math. Sci., 9: 997-1012, 2001.) to incorporate solitons with nontrivial phase profile.

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PP1

Detecting And Using Stable Communities For Modularity Maximization

Community detection through modularity maximization, is an important objective in large-scale network analysis. However, the value of the modularity and consequently the community membership is affected by vertex ordering of the network. We define a stable community as an invariant group of vertices that are always assigned to the same community. We present an algorithm to identify stable communities and show that combining stable communities as a preprocessing step leads to higher modularity. .

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PP1

Quantized Vortex Dynamics in Complex Ginzburg-Landau Equation in Bounded Domain

In this presentation, I will present efficient and accurate numerical methods for studying the quantized vortex dynamics and their interaction of the two-dimensional (2D) complex Ginzburg-Landau equation (CGLE) with a dimensionless parameter $\varepsilon > 0$ in bounded domains under either Dirichlet or homogeneous Neumann boundary condition. I will begin with a review of various reduced dynamical laws for time evolution of quantized vortex centers and show how to solve these nonlinear ordinary differential equations numerically. Then, I will present some results on the quantized vortex interaction under various different initial setup, and identify the cases where the reduced dynamical laws agree qualitatively and/or quantitatively as well as fail to agree with those from CGLE. Some other interesting phenomena will also be presented.

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PP1

Statistical Test and Simulation for Multi-Scale Computation of 2D Polymer Model

Multi-scale computation is an accurate and highly efficient computing method involving simulation and analysis of information at different resolutions. Due to its common applications, many mathematicians expect to ameliorate the level of accuracy and efficiency to an even higher level. One potential way is to analyze the statistics of data, and enhance the algorithm by knowing the trend of data. Here we discuss the statistical methods involving in 2D polymer model.

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PP1

An Analytical Approach to Green Oxidation

In this poster, we study the problem of suicidal inactivation of oxidation catalysts. We formulate a system of differential equations that models chemical reactions and analyze its numerical and analytical properties. Noticing its similarity with Michaelis-Menten system, we have been able to develop quasi-state approximation that together with perturbation techniques has allowed us to derive an approximate solution. The main goal is to estimate the rates of the reactions for deeper understanding of the system.

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PP1

Conditional Stochastic Simulations and Error Estimates for Flow and Transport in Porous Media

We use stochastic parameterizations to describe the properties of the coefficients of flow and transport model; then we use stochastic collocation or Monte Carlo simulations to solve the system of PDEs. The novelty is that we are able to include prior data for which conditional parameterizations are obtained. We provide comparison with unconstrained simulations. Additionally, we derive error estimates for the quantities of interest in the coupled system.

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PP1

A Method of Lines Approach to Solving Pdes on Surfaces

Partial differential equations (PDEs) posed on surfaces appear often in mathematical modelling. The Closest Point Method is a numerical technique for solving these types of equations, by embedding the surface in a higher-dimensional space. We present a new way to formulate an embedding equation which leads to a simple method of lines approach. We also include a variety of computational examples.

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PP1

Proper Orthogonal Decomposition Reduced Order Models For Complex Flows

Reduced-order models are frequently used in the simulation of complex flows to overcome the high computational cost of direct numerical simulations, especially for three dimensional nonlinear problems. Proper orthogonal decomposition is one of the most commonly used methods to generate reduced-order models for turbulent flows dominated by coherent structures. To balance the low computational cost required by a reduced-order model and the complexity of the targeted turbulent flows, appropriate closure modeling strategies need to be employed. In this paper, we will present several new nonlinear closure methods for proper orthogonal decomposition reduced-order models. We will also present numerical results for the new models used in realistic applications such as energy efficient building design and control, and climate modeling.

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PP1

Computing Positive Semidefinite Minimum Rank for Small Graphs

The positive semidefinite minimum rank (mr_+) of a simple graph G is the smallest possible rank over all positive semidefinite real symmetric matrices whose ijth (i not equal to j) entry is nonzero whenever ij is an edge, and zero otherwise. We programmed an implementation of known bounds in the open-source mathematical software Sage. The program, along with orthogonal representations, establishes mr_+ for all graphs of order 7 or less.

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PP1

Improving Hidden Markov Models that use Classified Observations

A Hidden Markov Model looks at observations generated by a "hidden" Markov process. When the observed data is complex, it must first be classified before it can be used in such a model. We use classification methods borrowed from natural language processing to prepare observation data to train a Hidden Markov Model. As an example we consider grouping clients based on health insurance claims.

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PP1

Improving Certainty Using Informed Markov Models

Hidden Markov Models are a powerful tool for analysis when a Markov Process is not directly observable. However, in a complicated model the sequence of observable states with maximum likelihood may have a probability very near to zero. We examine how these probabilities are affected as we add information to the model, either via the hidden Markov process, or through the observation probability matrix.

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PP1

Diversification Effect of Distributed Solar Energy Upon Energy Generation Volatility

High levels of volatility are a significant impediment to the integration of solar energy into the electric grid. Combining the output of geographically distributed solar systems results in a diversification effect that reduces the aggregated volatility. This diversification effect has been previously proposed, but it has undergone limited validation under controlled conditions. We have quantified and validated this diversification effect across a large fleet of distributed solar installations in the field using highly granular data.

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PP1

Restructuring the Ppm Gas Dynamics Algorithm for Many-Core Cpu Devicces

The latest CPU devices contain a large number of cores (over 50 on Intels new MIC processors) that all must work together in order to achieve the best performance. Techniques and tools for restructuring fluid dynamical computations to allow all the cores on a single CPU chip to work cooperatively on data that they share in the processor caches will be described, using the PPM gas dynamics algorithm as an example.

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PP1

A Radial Basis Function Partition of Unity Method for Transport on the Sphere

The transport process dominates geophysical fluid motions on all scales making the numerical solution of the transport problem fundamentally important for the overall accuracy of any flow solver. We present a new high-order, computationally efficient method for this problem that uses radial basis functions in a partition of unity framework. Results of the method are presented for several well-known test cases that probe the suitability of numerical methods for modeling transport in spherical geometries.

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PP1

Grain Boundaries in Turing Patterns

Our main results show the existence of grain boundaries, describe their shapes, and exhibit bifurcations where grain boundaries split into pairs of concave and convex disclinations. Our work is split into two parts. In the first part, we show that universally, for any pattern-forming system near onset, that is, for small-amplitude patterns, the shape of grain boundaries is determined by a system of coupled ordinary differential equations. Those equations are obtained by recently developed reduction theorems for ill-posed elliptic partial differential equations. The key observation is that those reduced equations are universal once put in normal form, that is, after a suitable change of coordinates. They contain only very few parameters and their solutions can be fully analyzed despite the fact that the dimension of the system of equations is at least 12, and tends to infinity when the angle between rolls becomes small.

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PP1

Parallel Cardiac Image Segmentation with Random Projection Tree

Due to noise, artifacts and high accuracy requirement, medical image segmentation is always a challenging problem. We proposed a data-driven approach, which classified each pixel based on the similarity along the low dimensional parameterization of the feature space. In particular, our framework discovers the intrinsic structure of high dimensional wavelet features using a random projection tree structure, which is built on top of MPI and OpenMP for massive dataset, and shows excellent scalability and speedup.

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PP1

Local Convergence of Newton-Type Methods for Degenerate Eigenvalues of Nonlinear Algebraic Eigenvalue Problems

We analyze the local convergence rates of several Newton-type methods for the computation of a semi-simple or defective eigenvalue of general nonlinear algebraic eigenvalue problems of the form $T(\lambda)v = 0$. We show that the convergence for semi-simple eigenvalues is similar to that for simple ones. For defective eigenvalues, Newton-type methods converge only linearly. A class of accelerated methods is proposed and shown to exhibit quadratic convergence.

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PP1

Computation of Harmonic Forms of the Vector Laplacian

The vector Laplacian arises in electromagnetics and other applications, and an important role is played by its null space, the space of harmonic forms. I present an algorithm to compute a basis of this space. The algorithm combines mixed finite elements for discretization, algorithms from computational geometry to analyze the topology, and a variation of the power method suitable for multiple eigenvalues. I also consider various ways to approximate localize the harmonic basis functions.

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PP1

AWM - A New Approach to Understanding the Dynamics of the Formation of Magnetic Domains

Traditionally, ferromagnetism is studied using the Ising model, which is exactly solvable in one or two dimensions and of limited use in the infinite- dimensional mean field case. While preserving the classic energy arguments, our model uses techniques previously applied to sociophysics to allow for arbitrary coupling between particles. By predicting the dynamics of the approach to magnetic equilibrium, we hope to improve the understanding of phase transitions in materials of various lattice structures.

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PP1

Partially Parallel Magnetic Resonance Image Reconstruction Using Bregmanized Operator Splitting with Variable Stepsize

This paper proposes a Bregman operator splitting algorithm with variable stepsize (BOSVS) for solving nonsmooth and nonlinear optimization problems of the form $\min_u\{\phi(\nabla u)+1/2\|Au-f\|_2^2\}$, where ϕ is a nonsmooth function. This algorithm uses a line search to achieve better efficiency. The stepsize rule starts with a Barzilai-Borwein (BB) step, and increases the nominal step until a termination condition is satisfied. Theoretically, this algorithm converges globally to the optimal solution of the optimization problem. Numerically, we get significantly better results compared to original BOS algorithm with fixed stepsize and SBB algorithm with BB stepsize. Experimental results in partially parallel magnetic resonance image reconstruction displays that BOSVS algorithm gives greater stability, accuracy and speed.

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PP1

Stochastic Simulation and Power-Law Relaxation of Highly Entangled Wormlike Micellar Solutions

Wormlike micelles, long flexible self-assembled aggregates of surfactant molecules, form entangled networks in solution. These mixtures exhibit two relaxation mechanisms, reptation and reversible breaking. Experiments in concentration regimes in which the worms are highly entangled show power law stress relaxation instead of the exponential relaxation predicted by most traditional models (Johnson-Segalman, Giesekus, VCM). In this poster, we present flow predictions, using stochastic simulations, to understand the mechanisms of the power-law relaxation regime.

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PP1

AWM - Min-Max Game Theory Problem for the Fluid-Structure Interaction Model: An Application to the Medicine Effect on Blood Flow in Human Body

The min-max game theory problem for the fluid-structure interaction model is considered. We apply the model to a biological scenario, where the medicine and the bacteria/viruses become two players counteracting on the blood flow and blood cells inside the human body. The motions of the blood flow and blood cells are described by Navier-Stokes equation and elastic equation respectively. Our goal is to find the optimal dose of the medicine for the patient that can kill worst possible bacteria/viruses in his body.

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PP1

How to Compute Transition States/saddle Points?

Exploring complex energy landscape is a challenging issue in many applications. Besides locating equilibrium states, it is often also important to identify transition states given by saddle points. In this talk, we will discuss existing and new algorithms for the computation of such transition states with a focus on the newly developed Shrinking Dimer Dynamics and present some related mathematical theory on stability and convergence. We will consider a number of applications including the study of frustrations of interacting particles and nucleation in solid state phase transformations.

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PP1

Multi-Layer and Multi-Resolution Large Population Stochastic Games

Game theory has been used to understand and design complex systems with many interacting independent decision-making agents in changing environments. In this work, we study a class of large population stochastic games with multi-layer (ML) and multi-resolution (MR) structures. We first look at ML games in which the players have hybrid dynamics where the continuous dynamics model the interactions at the physical layer of the system, and the discrete dynamics model the behavior at the cyber layer. In the second part of the work, we study MR games where players face competitions within their group as well as interact with members outside their groups through global parameters such as price, temperature, etc. We adopt a mean-field approach to characterize the mean-field Nash equilibria of ML and MR games. We apply the framework and results to study complex systems such as molecular transport and demand response in the smart grid.

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PP1

Dynamics and Noise Minimization of Femto-Second Similariton Pulses in a Fiber Laser with Zero Average Disperion

Various experimental designs have recently been proposed for ultra-short pulse mode-locked fiber lasers with applications to optical clocks, time and frequency transfer, generation of arbitrary optical waveforms, and frequency-comb spectroscopy. We will present simulation results (independently confirmed by laboratory experiments) demonstrating the existence of self-similar femto-second pulses near zero average dispersion in a laser with a Ytterbium fiber, and show that timing jitter is minimized when the average dispersion is close to zero.

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FM12 Abstracts

SIAM Conference on

Financial Mathematics & Engineering

July 9-11, 2012
Hyatt Regency Minneapolis
Minneapolis, Minnesota, USA

IC1

Optimal Execution in a General One-Sided Limit Order Book

We construct an optimal execution strategy for the purchase of a large number of shares of a financial asset over a fixed interval of time. Purchases of the asset have a nonlinear impact on price, and this is moderated over time by resilience in the limit-order book that determines the price. The limit-order book is permitted to have arbitrary shape. The form of the optimal execution strategy is to make an initial lump purchase and then purchase continuously for some period of time during which the rate of purchase is set to match the order book resiliency. At the end of this period, another lump purchase is made, and following that there is again a period of purchasing continuously at a rate set to match the order book resiliency. At the end of this second period, there is a final lump purchase. Any of the lump purchases could be of size zero. A simple condition is provided that guarantees that the intermediate lump purchase is of size zero. This is joint work with Gennady Shaikhet and Silviu Predoiu.

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IC2

Stable Diffusions With Rank-based Interactions, and Models of Large Equity Markets

We introduce and study ergodic diffusion processes interacting through their ranks. These interactions give rise to invariant measures which are in broad agreement with stability properties observed in large equity markets over long time-periods. The models we develop assign growth rates and variances that depend on both the name (identity) and the rank (according to capitalization) of each individual asset. Such models are able realistically to capture critical features of the observed stability of capital distribution over the past century, all the while being simple enough to allow for rather detailed analytical study. The methodologies used in this study touch upon the question of triple points for systems of interacting diffusions; in particular, some choices of parameters may permit triple (or higher-order) collisions to occur. We show, however, that such multiple collisions have no effect on any of the stability properties of the resulting system. This is accomplished through a detailed analysis of collision local times. The models have connections with the analysis of Queueing Networks in heavy traffic, and with competing particle systems in Statistical Mechanics (e.g., Sherrington-Kirkpatrick model for spin-glasses). Their hydrodynamic-limit behavior is governed by generalized porous medium equations with convection, whereas limits of a different kind display phase transitions and are governed by Poisson-Dirichlet laws.

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IC3

Simulation Schemes for Stopped Lvy Processes

Jump processes, and Lvy processes in particular, are notoriously difficult to simulate. The task becomes even harder if the process is stopped when it crosses a certain boundary, which happens in applications to barrier option pricing or structural credit risk models. In this talk, I will present novel adaptive discretization schemes for the simulation of stopped Lvy processes, which are several orders of magnitude faster than the traditional approaches based on uniform discretization, and provide an explicit control of the bias. The schemes are based on sharp asymptotic estimates for the exit probability and work by recursively adding discretization dates in the parts of the trajectory which are close to the boundary, until a specified error tolerance is met.

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IC4

Talk Title TBA - Avellaneda

Abstract not available at time of publication.

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IC5

Optimal Order Placement in Limit Order Books

Abstract not available at time of publication.

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IC6

Quantitative Absence of Arbitrage and Equivalent Changes of Measure

It is well known that absence of arbitrage is a highly desirable feature in mathematical models of financial markets. In its pure form (whether as NFLVR or as the existence of a variant of an equivalent martingale measure R), it is qualitative and therefore robust towards equivalent changes of the underlying reference probability (the "real-world" measure P). But what happens if we look at more quantitative versions of absence of arbitrage, where we impose for instance some integrability on the density dR/dP? To which extent is such a property robust towards changes of P? We discuss these questions and present some recent results. The talk is based on joint work with Tahir Choulli (University of Alberta, Edmonton).

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SP1

AWM-SIAM Sonia Kovalevsky Lecture : The Role of Characteristics in Conservation Laws

Sonya Kovalevsky, in the celebrated Cauchy-Kovalevsky theorem, made clear the significance of characteristics in partial differential equations. In the field of hyperbolic conservation laws, characteristic curves (in one space dimension) and surfaces (in higher dimensions) dominate the behavior of solutions. Some examples of systems exhibit interesting, one might even say pathological, characteristic behavior. This talk will focus on ways that characteristics in systems of conservation laws give information about the systems being modeled.

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SP2

The John Von Neumann Lecture: Liquid Crystals for Mathematicians

Liquid crystals form an important class of soft matter systems with properties intermediate between solid crystals and isotropic fluids. They are the working substance of liquid crystal displays, which form the basis of a huge multinational industry. The lecture will describe these fascinating materials, and what different branches of mathematics, such as partial differential equations, the calculus of variations, multiscale analysis, scientific computation, dynamical systems, algebra and topology, can say about them.

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SP3

Past President's Address: Reflections on SIAM, Publishing, and the Opportunities Before Us

Upon taking up the post of president I had, of course, formulated my priorities for SIAM. This talk provides a good occasion to revisit some of those. One area turned out to play a vastly larger role than I would have anticipated, namely mathematical publishing and many issues associated with it, ethical, technological, economic, political, and scientific. The future of scholarly publishing is far from clear, but one thing seems certain: big changes are needed and will be coming. We, as mathematicians, are major stakeholders. We should also be major agents in guiding these changes. I will present some of my observations and thoughts as we confront the opportunities before us.

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SP4

W. T. and Idalia Reid Prize Lecture: Large Algebraic Properties of Riccati Equations.

In the eighties there was considerable interest in the algebraic properties of the following Riccati equation

$$A^*X + XA - XBB^*X + C^*C = 0, \quad (1)$$

where $A, B, C \in A$, a Banach algebra with identity, and the involution operation $*$. Conditions are sought to ensure that the above equation has a solution in A. The results were disappointing and the problem was forgotten until this century when engineers studied the class of spatially distributed systems. One application was to control formations of vehicles where the algebraic property was essential. This case involves matrices A, B, C with components in a scalar Banach algebra. Positive results are obtained for both commutative and noncommutative algebras.

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SP5

I.E. Block Community Lecture: Creating Reality: the Mathematics Behind Visual Effects

Abstract to follow.

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SP6

SIAG/FME Junior Scientist Prize: Market-Based Aapproach to Modeling Derivatives Prices

Most of the existing quantitative methods in Finance rely on the assumptions of the underlying mathematical models. The problem of choosing the appropriate model assumptions is one of the cornerstones of modern Financial Engineering. I am interested in developing modeling frameworks that facilitate the use of historical observations when making the choice of model assumptions. It turns out that, in the markets with a large family of liquid derivative contracts, it is rather hard to construct a model that exploits the information contained in the historical prices of these derivatives. In fact, constructing such models requires the use of the so-called Market-Based Approach. The idea of this approach is to treat the liquid derivatives as generic financial assets and prescribe the joint evolution of their prices in such a way that any future arbitrage-free combination of prices is possible. In this presentation, I will outline the main difficulties associated with the construction of market-based models and will present a general methodology that bypasses these difficulties. Finally, I will illustrate the theory by describing (both mathematically and numerically) a family of market-based models for the European call options of multiple strikes and maturities.

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JP1

Systemic Risk

What is systemic risk, how do we model it, how to we analyze it, and what are the implications of the analysis? I will address these issues both in a larger historical context and within current research mathematical finance. The key property of systems subject to systemic risk is their interconnectivity and the way individual risk can become overall, systemic risk when it is diversified by inter-connectivity. I will discuss theoretical issues that come up with mean-field and other models and will also show results of numerical simulations.

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CP1

Pricing Interest Rate Derivatives in a Multifactor Hjm Model with Time Dependent Volatility

We investigate the partial differential equation (PDE) for pricing interest rate derivatives in a multi-factor Cheyette Model, that involves time-dependent volatility functions with a special structure. The high dimensional parabolic PDE that results is solved numerically via a sparse grid approach, that turns out to be both accurate and efficient. The results are compared to the analytical solution for bonds and caplets and also the Monte Carlo simulation solution for Bermudan Swaptions.

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CP1

A Paradigm Shift in Interest-Rate Modeling

This research starts with a solution for modeling nonnegative interest rates in an incomplete bond market. It is the *stochastic-splines model*, in which instantaneous forward rates are almost surely finite and approximately lognormal under both the real-world and the risk-adjusted measures. A unique term structure of convenience yield for the default-free bond market is introduced for the first time to compensate idiosyncratic risk. Addressing on the market completeness issue, the *stochastic-volatility stochastic-splines model* is presented whereby bond convenience yield vanishes. Under this framework, the market price of volatility risk can be computed endogenously. Various applications are given.

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CP1

Pricing Swaptions under Multifactor Gaussian Hjm Models

Several approximations have been proposed in the literature for the pricing of European-style swaptions under multifactor term structure models. However, none of them provides an estimate for the inherent approximation error. Until now, only the Edgeworth expansion technique of Collin-Dufresne and Goldstein (2002) is able to characterize the order of the approximation error. Under a multifactor HJM Gaussian framework, this paper proposes a new approximation for European-style swaptions, which is able to bound the magnitude of the approximation error and is based on the *conditioning approach* initiated by Curran (1994) and Rogers and Shi (1995). All the proposed pricing bounds will arise as a simple by-product of the Nielsen and Sandmann (2002) setup, and will be shown to provide a better accuracy-efficiency trade-off than all the approximations already proposed in the literature.

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CP1

Pricing and Hedging the Smile with Sabr: Evidence from the Interest Rate Caps Market

This is the first comprehensive study of the SABR (Stochastic Alpha-Beta-Rho) model (Hagan et. al (2002)) on the pricing and hedging of interest rate caps. We implement several versions of the SABR interest rate model and analyze their respective pricing and hedging performance using two years of daily data with seven different strikes and ten different tenors on each trading day. In-sample and out-of-sample tests show that in addition to having stochastic volatility for the forward rate, it is essential to recalibrate daily either the vol of vol or the correlation between forward rate and its volatility, although recalibrating both further improves pricing performance. The fully stochastic version of the SABR model exhibits excellent pricing accuracy and more importantly, captures the dynamics of the volatility smile over time very well. This is further demonstrated through examining delta hedging performance based on the SABR model. Our hedging result indicates that the SABR model produces accurate hedge ratios that outperform those implied by the Black model.

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CP2

Swing Options in Commodity Markets: A Model with Multidimensional Jump Diffusions

The objective of this talk is to study the optimal exercise policy of a swing option in the electricity markets. We formulate a model in terms of a stochastic control problem in continuous time, subjected to a total volume constraint. The underlying price process is a linear function depending on a multidimensional Lévy diffusion. The results are illustrated with examples.

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CP2

Decomposing the Risk from Investing in Foreign

Commodities

Several papers show that FX rates and commodity prices are interlinked. When investing in commodities traded in a foreign currency, the investor faces both price risk and FX risk. We investigate how exchange-traded contracts on WTI crude oil and EUR/USD correlate. We propose and estimate a model that accounts for the stochastic correlation between the two. This can be used to price and risk manage foreign commodity positions, e.g., quanto options or oil-linked gas contracts.

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CP2
A Real-Time Pricing Model for Electricity Consumption

Input your abstract, including TeX commands, here. The California electric company, i.e., PGE (Pacific Gas and Electric Co.,), has recently announced its intentions to charge small businesses in the state with dynamic prices for electricity consumption. In this regard, we study a real-time electricity pricing model in the paper and compare it with two static pricing models. We show that real-time pricing outplays static pricing when it comes to jointly maximizing provider and consumer welfare.

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CP2
A Resampling Particle Filter Parameter Estimation For Electricity Prices With Jump Diffusion

In this paper we propose a particle ?lter for parameter estimation of jump diffusion models employed for modelling electricity prices 1,2,3,4,5. We consider a jump-diffusion model 4. The jumps has the possibility to give a better explanation of the behaviour of electricity prices, however estimation of parameters becomes more complicated 4.Complications in parameter estimation will be introduced by the inclusion of the jump component. The inclusion of jumps will add several new parameters 4. These parameters will describe the jump frequency and distribution. The jump models are non-Gaussian and this increases the complexity of the models 1,2,3,4. A known ?ltering technique for these models is particle ?lter 1,2,3. Particle ?lter (PF) is a fully non-linear ?lter with Bayesian conditional probability estimation, compared here with the well-known ensemble Kalman lter (EnKF). A Gaussian resampling (GR) method is proposed to generate the posterior analysis ensemble in an effective and efficient way 3. The performance of gaussian particle ?lter to model the jump frequency and distribution parameters will be investigated and benchmarked to other maximum likelihood state estimators.

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CP3
Basket and Spread Options in a Variance Gamma Model

Financial asset returns exhibit higher skewness and kurtosis than those implied by the Normal distribution. Price paths can also exhibit jumps, which is particularly true for emerging and commodity markets. In this case, the Variance Gamma (VG) process is more realistic than the geometric Brownian motion (GBM) to model the asset price dynamics. However, valuation of basket and spread options (common derivatives in commodity, FX and other markets) under this model is a very challenging and time-consuming task. We propose a novel and elegant method for valuation of basket and spread options under VG model, by conditioning the VG processes on a realization of the stochastic Gamma time change and combining it with the Generalized LogNormal (GLN) approximation. We consider a simpler (and easily tractable) case of the identical stochastic time change for all underlying assets, as well as the more general case of dierent (but dependent) Gamma time changes. Numerical study shows that the proposed method performs remarkably well in term of option pricing, even for a simpler model. Our method is intuitive, computationally very fast, ecient and exible enough to allow for basket options on arbitrary number of assets and negative portfolio weights.

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CP3
High-order Short-time Expansions for ATM Option Prices Under the CGMY Model

In this presentation, we derive a novel second-order approximation for ATM option prices under the CGMY Lvy model, and then extend to a model with an addition Brownian motion. The third-order asymptotic behavior of the option prices as well as the asymptotic behavior of the corresponding Black-Scholes implied volatilities are also addressed. Our numerical results show that in most cases the second-order term significantly outperform the first order approximation.

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CP3
Efficiently Simulating the Double-Barrier First-Passage Time in Jump-Diffusion Models

We present a fast and accurate Monte-Carlo simulation to obtain double-barrier first-passage time probabilities in a jump-diffusion model with arbitrary jump size distribution; extending single-barrier results by Metwally and Atiya [2002]. The presented algorithm is unbiased and significantly faster than a brute-force Monte-Carlo simulation on a grid. As an application, we discuss corridor bonus certificates, floor certificates, and digital first-touch options.

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CP3

Numerical Solution of Jump-Diffusion SDEs

Jump-diffusions are ubiquitous in finance and economics. This paper develops, analyzes and tests a discretization scheme for multi-dimensional jump-diffusion SDEs with general state-dependent drift, volatility, and jump intensity function. Unlike conventional schemes, our scheme allows for an unbounded jump intensity–a feature of many standard jump-diffusion models in credit, equity, FX and commodity markets. The convergence of the discretization error is proved to be of weak order one. Numerical experiments illustrate our results.

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CP4

Model Risk Based on the Distribution of the Hedge Error

When pricing and hedging a derivative, we face model risk, that is, the risk of choosing the wrong dynamics for the financial market. We propose a measure of model risk based on the hedge error that can be interpreted as a capital charge. This has several positive implications beyond estimating the riskiness of a claim in terms of model risk. We calculate these model risk measures for several examples and derive its general properties.

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CP4

Why Is It So Hard to Estimate Expected Returns?

A key part of experiment design is determining how much data to collect. When the data comes in the form of a timeseries, the sample size is expressed both by the count N of the observations and the duration T of the historical period over which observations were made. For an asset whose price has continuous sample paths, we demonstrate that the standard error of any unbiased estimator of the price of risk is bounded below by $1/\sqrt{T}$.

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CP4

A New Perspective on Dependence Within Financial Markets

Many financial instruments are inherently multivariate in their origination. A rigorous empirical valuation requires simultaneous analysis of many components. Nonlinear and inter-temporal dependencies, extreme events, and large datasets introduce additional challenges. Independent component analysis is an indispensable tool for finding suitable representations of the complex multivariate information within financial markets. We introduce a novel statistical framework for independent component analysis of financial data and illustrate its use on several important financial applications.

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CP4

The Herd Behavior Index: a New Measure for the Implied Degree of Co-Movement in Stock Markets

We introduce a new measure for the implied degree of herd behavior, one of the driving factors of systemic risk. This forward looking Herd Behavior Index (HIX) is model-independent and based on observed option data. As an illustration, we determine historical values of the 30-days HIX for the Dow Jones Industrial Average.

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CP5

Incorporating Parameter Risk into Derivatives Prices - An Approach to Bid-Ask Spreads

We present a new method based on convex risk measures to incorporate parameter risk (e.g. estimation and calibration risk) into derivative prices. As an application we calculate parameter risk-implied bid-ask spreads of exotics, enabling us to compare the parameter risk of different models and different exotics. Furthermore, we introduce a nonparametric calibration procedure to real bid-ask prices using distortion risk measures, compare our results to given parametric distortion calibrations and present a new parametric family.

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CP5

Analytical Calculation of Risk Measures for Vari-

able Annuity Guaranteed Benefits

With the increasing complexity of investment options in life insurance, more and more insurers have adopted stochastic modeling methods for the assessment and management of insurance and financial risks, with the most prevalent being Monte Carlo simulation. In this paper we propose an alternative analytical method for the calculation of risk measures for variable annuity guaranteed benefits. The techniques for analytical calculations are based on the study of an integral of geometric Brownian motion as well as asymptotic analysis of special functions. As we demonstrate by numerous examples on quantile risk measure and conditional tail expectation, the numerical algorithms developed in this paper appear to be accurate and computationally efficient.

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CP5
Fair Valuation of Drawdown Insurance

Drawdowns are path-dependent measures of risk and have been used extensively in the description of market crashes. We evaluate the market price of a market crash as measured through drawdowns by considering an investor who wishes to insure herself against the risk of a market crash and does so by purchasing insurance claims against drawdowns. We further examine the fair valuation of drawdown insurance in the possibility of early cancellation and identify optimal cancellation strategies.

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CP5
Diversification and Crash-Protection Using Variance Swap Calendar Spreads

Volatility can be also considered an asset class. Variance swaps, one of the main investment vehicles, provide exposure to realized volatility. Implied volatility is often higher than the realized volatility will turn out to be. We explain how a variance swap calendar spread benefits from both negative risk premium and negative correlation with the underlying stock index. Via backtesting we show how the strategy added to a stock/bond portfolio significantly diversifies crash risk.

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CP6
Optimal Cash Holdings in a Firm

The precautionary principle of cash-holdings is empirically well analysed. However, the quantitative modelling of such cash holdings is exceptionally sparse. This is due to the path dependent nature of the problem and the fact that cash holdings may both increase and decrease in time. As such, novel numerical solutions to the problem are required. We show how to model endogenous cash holdings within a Firms valuation and extract numerical solutions. In doing so we provide a solid basis by which Real Options analysis, dividend payments, debt issuance, cash holdings, and corporate finance decisions (investments) can finally all be viewed in a consistent, non-contradictory and more realistic fashion. This analysis and need for consistency has been called for within many papers, and we hope our (economically robust) approach shows how mathematics can provide a more unifying approach to the theory of the Firm.

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CP6
Risk Aversion and Managerial Cash-Flow Estimates in Real Options

While there are a number of academic papers discussing the importance of accounting for risk aversion in real option valuation, none of them are applicable to discrete cash-flow estimates supplied by managers. Here, we develop an approach which explicitly incorporates managerial cash-flow estimates and accounts for risk-aversion through indifference valuation. Interestingly, we find that the real option value not only deteriorates as risk-aversion increases, it drops to zero above a critical risk-aversion level.

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CP6
Irreversible Investment with Regime Switching : Revisit with Linear Algebra

We consider irrevesible investment problems with regime switching feature under a monopoly setting. Several parameters describing the economic environment varies according to a regime switching with general number of states. We present the derivation of the value function via solving a system of simultaneous ordinary differential equations with knowledge of linear algebra. It is found that the functional form of the value function depends on the decomposition of a coefficient matrix.

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CP6

Embedded Currency Exchange Options in Roll-over Loans

In ship and aircraft financing long term roll-over loans are often equipped with the right to change the currency every quarter at spot. The loan taker then pays LIBOR of the respective currency plus a pre-determined constant sales margin. If the capital outstanding exceeds 105% calculated in the original currency, the amortization is required to the level of 105% of the original currency. By clever currency management the loan taker can amortize the loan faster and terminate the loan early. Essentially the loan taker owns a series of options on the cross currency basis spread with unknown notional amounts. We determine the key drivers of risk, an approach to valuation and hedging, taking into consideration the regulatory constraints of a required long term funding. We present a closed-form approximation to the pricing problem and illustrate its stability.

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CP7

Dynamic Quadratic Hedging in the Presence of Partially Hedgeable Assets and Liabilities

We consider an incomplete market where an investor who owns a partially hedgeable asset faces a liability at time T. The investor's aim is to minimize the terminal replication error based on a quadratic loss criterion in this setting. We investigate the solution to the quadratic hedging problem using the stochastic linear-quadratic optimal control approach through the corresponding (stochastic Riccati) BSDEs and provide some examples.

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CP7

BSDEs with BMO Market Price of Risk

We study quadratic semimartingale BSDEs arising in power utility maximization when the market price of risk is of BMO type. In a Brownian setting we provide a necessary and sufficient condition for the existence of a solution but show that uniqueness fails to hold in the sense that there exists a continuum of distinct square-integrable solutions. This feature occurs since, contrary to the classical Ito representation theorem, a representation of random variables in terms of stochastic exponentials is not unique. We study when the BSDE has a bounded solution and derive a new dynamic exponential moments condition which is shown to be the minimal sufficient condition in a general filtration. The main results are complemented by several interesting examples which illustrate their sharpness as well as important properties of the utility maximization BSDE.

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CP7

A Continuous Time Bank Run Model for Insolvency, Recovery and Rollover Risks

We propose a continuous time bank run model for incorporating insolvency, recovery and rollover risks. The firm finances by issuing both long and short term debt, and the short term debt holders need to decide whether to roll over or to withdraw their debt (i.e. to run the bank) when their contracts expire. We show there exists a threshold strategy (i.e. the bank run barrier) for the short-term creditors to decide when to run. We decompose the total credit risk into an insolvency component and an illiquidity component based on such an endogenous bank run barrier together with an exogenous insolvency barrier. The short term debt in our model can have either a discrete tenor structure, or a more realistic staggered tenor structure. The problem is reduced to an optimal stopping time problem with constraint, which is solved by the BSDE method.

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CP7

Quadratic Reflected Bsdes with Bounded Conditions. Application to American Options.

In this talk, I present an elementary and totally perturbative method for dealing with the well-posedness of some reflected BSDEs : existence, uniqueness and stability. It works for a smooth coefficient f which has a growth at most quadratic in z, when the terminal condition as well as the lower obstacle are bounded. I then connect these equations with the problem of pricing american options in an incomplete market.

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CP7

A Simple Proof of BichtelerDellacherieMokobodzki Theorem

We give a simple and quite elementary proof of the celebrated BichtelerDellacherieMokobodzki Theorem, which states that a process is a good integrator if and only if it is a semi-martingale. Moreover we reformulate its statement in a way that -we believe- is more natural.

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CP8

Inference for the Fractional Heston Model Using the Auxiliary Particle Filter

The fractional Heston Model is a generalization of the Heston Model obtained by replacing Brownian motion by fractional Brownian motion in the two equations that define the Heston model. After defining the fractional Heston model and showing its representation as a Dynamic state space model, we will use that auxiliary particle filter both to sample the volatility process and to update the posterior distribution of the parameters sequentially as data arrive over time. We apply our approach to simulated and real data with success. Keywords:- Fractional Heston Model, maximum likelihood estimation, particle filter, auxiliary particle filter, sequential Bayesian inference.

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CP8

Non-Parametric Calibration of the Local Volatility Surface for European Options

Assuming the volatility surface is smooth, a second order Tikhonov regularization is applied to the calibration problem. Additionally a new approach for choosing the Tikhonov regularization parameter is proposed. Using the TAPENADE automatic differentiation tool in order to obtain adjoint code of the direct model is employed as an efficient way to obtain the gradient of cost function with respect to the local volatility surface. Finally we perform four numerical tests aimed at assessing and verifying the aforementioned techniques.

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CP8

Small-time Asymptotics For Some Stochastic Volatility Models

In the paper SMALL-TIME ASYMPTOTICS FOR FAST MEAN-REVERTING STOCHASTIC VOLATILITY MODELS they investigate two rates for the mean-reversion time δ in terms of the maturity ϵ, namely $\delta = \epsilon^{\gamma}$ for $\gamma = 2, 4$. Looking at this model and a few others we characterize the behaviors for $\gamma > 2$ and for $1 < \gamma < 2$ and show how this relates to Moderate Deviations and Super-large Deviations, respectively. This argument also shows why $\gamma = 2$ is special.

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CP8

Stochastic Calibration to Implied Volatility Surfaces

This paper provides a two-step method to fully calibrate the implied volatility surface in the environment of random volatility. The first step consists of the Fourier transform method (Malliavin and Mancino (2009)) for estimating model parameters of stochastic volatility models, and the second step solves an optimization problem by means of Monte Carlo simulation with variance reduction techniques. We compare fitting accuracies with the fast Fourier transform method (Carr and Madan (1999)) and perturbation method (Fouque et al. (2003, 2011)). In addition, it is natural to generalize our calibration procedure to the implied volatility surface of American options.

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CP8

Understanding Jumps in the High-Frequency VIX

This article provides a comprehensive nonparametric high-frequency analysis of jumps in the VIX (S&P500 volatility index). A comparison of the VIX and the S&P500 futures time series (1992-2010) shows that 97% of jumps in the VIX are spurious. This finding not only leads to a new interpretation of the broadly used VIX dataset but also extends the literature on volatility jumps and on the return-volatility relationship.

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CP8

Implied Volatiltiy from Black-Scholes and Other Formulas

We show that if the parameters of an arbitrary stock price model are used in the Black-Scholes formula for calculating option prices for finitely many strikes, the implied volatility (a function of time t) will be bounded by a value which depends only on strikes. Our model-free results, which can be used in calibration, provide sets of constraints limiting the acceptable values of the implied volatility parameters. We use the Heston model for illustration.

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CP9

Extensions of the Lt Method for Option Pricing

Monte Carlo (MC) and quasi-Monte Carlo (QMC) methods are often used in pricing complex derivatives. The merit of QMC is that, theoretically at least, higher convergence rates can be obtained than regular MC. The payoff function is usually high-dimensional and non-smooth, eliminating the advantage of using QMC. Imai & Tan (2006) introduced the LT method which minimizes the effective dimension of the problem by transforming the normal variates using an orthogonal transformation, thereby improving the QMC method. We extended their method for valuing options that have a barrier feature on an underlying asset, incorporating and extending an idea from Staum & Glasserman (2001). These options have a payoff that depends on whether the asset does or does not cross a certain level during the life of the option. If the probability of (not) hitting is large enough, then much more paths have to be sampled for reliable results. Our method greatly reduces the required number of paths and our aim is to extend this method to Levy market models.

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CP9

Variance Reduction for Monte Carlo Simulation of European Call Options Under the Coupled Additive-Multiplicative Noise Model

We propose a variance reduction method for Monte Carlo computation of option prices in the context of the Coupled Additive-Multiplicative Noise model. Four different schemes are applied for the simulation. The methods select control variates which are martingales in order to reduce the variance of unbiased option price estimators. Numerical results for European call options are presented to illustrate the effectiveness and robustness of this martingale control variate method.

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CP9

Central Limit Theorem for the Multi-Level Monte Carlo Algorithm and Applications to Option Pricing

This paper deals with the problem of the multi-level Monte Carlo method, introduced by Giles (Multilevel Monte Carlo path simulation Operations Research, 2008; 56:607-617) as an extended method of the statistical Romberg one introduced by Kebaier (Romberg Extrapolation: A New Variance Reduction Method and Applications to Option Pricing. Ann. Appl. Probab. 15 (2005), no. 4, 2681-2705). When approximating the expected value of a function of a stochastic differential equation solution, these methods improve efficiently the computational complexity of standard Monte Carlo. In this work, we analyze the asymptotic error of this algorithm and establish a central limit theorem based on a new stable functionalcentral limit theorem on the error in the Euler scheme for a given level. This allows us to obtain the optimal choice of the parameters method.Then, weinvestigate the application of this method to the pricing of Asian options. In this setting, the approximation relies on the discretization of the integral of the price process over a time interval. We also analyze the error process and prove a stable functional central limit theorem. Finally, We use our result in order to optimize the choice of the parameters, which are different from the ones in the Euler scheme. Numerical simulations were processed.

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CP9

A Hybrid Pricing Method for Options with Multi Assets

A numerical method is studied for options with multi-underlying assets. Instead of imposing artificial boundary condition for the multi-dimensional Black-Scholes equation, we calculate certain one-dimensional model equation at each time-step using pre-simulated Monte-Carlo time series. With standard finite difference method using nine point stencil, our method reduce the computational domain of the governing equation (the two dimensional Black-Scholes equation) exceedingly. As benchmark tests, we consider the call on the maximum option which has an analytic solution, and a complicated structured note from the derivative market.

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CP9

Control Variate Methods and Applications in Asian and Basket Options Pricing and Hedging under Jump-Diffusion Models

We discuss control variate methods with applications to Asian and basket option pricing under exponential jump diffusion models for the underlying asset prices. We first revisit the single control variate method and then discuss the multivariate control variate method in detail. Conditions which ensure the variance of an $m-$variate control variates is smaller than that of a $k-$variate control variates ($1 \leq k < m$) are given and proved. Based on these conditions, more efficient control variates can be constructed. For arithmetic Asian and basket options, control variates conditional on geometric means of asset prices are constructed. Numerical results show that the constructed control variate is much more efficient than the classical control variate when pricing Asian options even in high dimensional cases.

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CP9

Taylor-Like Anova Expansion for High Dimensional Pdes Arising in Finance

The solution of high dimensional problems in short time as well as with high precision is of great importance in finance. For this purpose we propose an approximation to an ANOVA decomposition of the problem, which is only of linear order in the dimension of the full problem and superior in precision. We will call this approximation Taylor-like ANOVA. We develop this approximation up to higher orders and show its efficiency by numerical experiments.

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CP10

Optimal Order Routing in Limit Order Markets

When executing a trade, traders in electronic equity markets can choose to submit a limit order or a market order, as well as the venue to submit this order, if the stock is traded in several exchanges. This decision is influenced by the order flow characteristics and queue sizes in each limit order book, as well as the structure of transaction fees and rebates across exchanges. We show that this optimal order routing problem may be formulated as a convex optimization problem and propose a stochastic algorithm for solving it. We study this problem under various statistical assumptions on the order flow and show the interplay between the fee structure, the order flow and the risk preferences of the trader in determining the optimal routing decision.

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CP10

Optimal Trade Execution with Dynamic Risk Measures

We propose a model for optimal trade execution in an illiquid market that minimizes a coherent dynamic risk of the sequential transaction costs. The prices of the assets are modeled as a discrete random walk perturbed by both temporal and permanent impacts induced by the trading volume. We show that the optimal strategy is time-consistent and deterministic if the dynamic risk measure satisfies a Markovian property. We also show that our optimal execution problem can be formulated as a convex program, and propose an accelerated first-order method that computes its optimal solution. The efficiency and scalability of our approaches are illustrated via numerical experiments.

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CP10

An Optimal Trading Rule under Switchable Mean Reversion Market

This work provides an optimal trading rule that allows buying or selling of an asset whose price is governed by mean-reversion model. In the model, the equilibrium level is controlled by an 2-state Markov chain. With the slippage cost imposed, the goal is to maximize the overall return. The value functions are characterized by considering the associated HJB equations. This paper also shows that the solution of the original optimal problem can be obtained by solving four quasi-algebraic equations. Finally, numerical examples are given for demonstration.

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CP10

Price Impact and Market Indifference Prices with Power Utilities

We investigate the price impact of large transactions in an equilibrium pricing model with HARA utility functions. A market maker trades with a large investor at a price that allows him to preserve his expected utility, the so-called market indifference price. In this setting we look at marginal prices and illiquidity premia in comparison to the Black-Scholes model as well as hedging and replication of non-traded (OTC) claims.

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CP10

A Self-exciting Point Process Model for Limit Order Books

The statistical properties of events affecting a limit order book -market orders, limit orders and cancellations- reveal strong evidence of clustering in time, significant cross-correlation across event types and significant dependence of the order flow on the bid-ask spread. We show that these dependencies may be adequately represented by a multi-dimensional self-exciting point process, for which a tractable parameterization is proposed. Using high-

frequency data from the Trades and Quotes database, we perform a Maximum Likelihood Estimation of the model and assess its predictive performance for a variety of stocks.

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CP10

Evolutionary Game Dynamics Using a Non-Equilibrium Price Formation Rule for Trading with Market Orders

Markets have dynamics that may result in excess volatility and other phenomena that are a challenge to explain using rational expectation models. Following Farmer (2002) and identifying trading strategies with species and capital invested in a strategy with a population, we use the replicator equation to identify the evolutionary game dynamics between the relevant agents. We then extend the dynamics spatially in order to examine the progression toward market efficiency caused by the evolution of capital. We observe interesting dynamics including the phenomenon that the market becomes efficient as new strategies find them and cause them to disappear.

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CP11

On the Existence of Shadow Prices.

For utility maximization problems under proportional transaction costs, it is known that the original market with transaction costs can sometimes be replaced by a frictionless shadow market that yields the same optimal strategy and utility. In this paper we present a counterexample which shows that shadow prices may fail to exist. We then prove that short selling constraints are a sufficient condition for their existence, even in very general multicurrency market models with discontinuous bid-ask-spreads.

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CP11

Indifference Pricing with Uncertainty Averse Preferences

We consider the indifference valuation of an uncertain monetary payoff from the perspective of an uncertainty averse decision-maker. We study how the indifference valuation depends on the decision-maker's attitudes toward uncertainty. We obtain a characterization of comparative uncertainty aversion and various characterizations of increasing, decreasing, and constant uncertainty aversion.

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CP11

Portfolio Optimization Based on Independent Sets of Market Cliques

We consider the problem of selecting an optimal market portfolio that maximizes expected return and includes highly correlated disjoint market cliques (i.e., members within a clique are pairwise highly correlated) which are pairwise anticorrelated based on a correlation function defined on the set of cliques. We present integer programming models that can be effectively used to construct such an optimal portfolio that satisfies given clique correlation thresholds.

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CP11

Portfolio Optimization under Convex Incentive Schemes

We consider the utility maximization problem of terminal wealth from the point of view of a portfolio manager paid by an incentive scheme given as a convex function g of the terminal wealth. The manager's own utility function U is assumed to be smooth and strictly concave, however the resulting utility function $U \circ g$ fails to be concave. As a consequence, this problem does not fit into the classical portfolio optimization theory. Using duality theory, we prove wealth-independent existence and uniqueness of the optimal wealth in general (incomplete) semimartingale markets

as long as the unique optimizer of the dual problem has a continuous law. In many cases, this fact is independent of the incentive scheme and depends only on the structure of the set of equivalent local martingale measures. We provide explicit examples for complete and incomplete market models.

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CP11
Optimal Portfolios for Hedge Funds and Their Managers

Hedge fund managers receive fees proportional to profits, and may reinvest them. We find the fund and personal portfolio that maximize managers' expected utility from personal wealth, when relative risk aversion is constant, and investment opportunities constant and separate, but correlated. Managers do not reinvest fees, allocating excess personal wealth in Merton portfolio. But they manage funds like Merton investors with risk aversion shrunk towards one. Managers do not hedge fund exposure with personal positions.

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CP11
An Equilibrium Approach to Utility-Based and Indifference Pricing

The utility-based and utility indifference pricing are frameworks for pricing contingent claims. Since these principles are based on utility maximization principle, prices are optimal for each investor with utility function. Our purpose is to expand these frameworks for deducing the equilibrium price. Another purpose is to clarify the relationship between utility-based and utility indifference framework. This discussion will be also done in the setting of the market with transaction costs.

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CP12
Optimal Decumulation: An Investment-Consumption Models for Retirees

We consider the optimal investment-consumption problem for retirees with uncertain lifespan. We assume that their initial wealth can spread between both risky and riskless (liquid) investments and an income-producing (irrevocable) life annuity with default risk. We examine whether default risk (or the perception of default risk) rationally affects a retirees decision to purchase an annuity upon retirement. We formulate our problem as a Hamilton-Jacobi-Bellman equation and do a thorough numerical study for CRRA investors.

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CP12
Voluntary Retirement and Annuity Contract

We consider an optimal financial planning problem of an economic agent who has an option to retire from labor voluntarily. The economic agent with labor income determines his/her investment strategy, consumption, and retirement strategy along with annuity. We investigate the relation between the annuity contract and the condition for the voluntary retirement. We also analyze how the presence of voluntary retirement option affects the purchase of an annuity and the annuity market.

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CP12
Bang-Bang Controls on Some Optimal Insurance Problems

In this talk, we are interested in finding an optimal solution for a large class of optimal insurance problems. This class of problems includes those whose risks are measured by Value at Risk, Average Value at Risk, Conditional Tail Expectation and law-invariant convex risk measures. We have found that Bang-Bang controls are optimal to all of them. This result also holds for multi-dimensional optimal insurance problems such as those in adverse selections.

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CP12
Optimal Consumption and Portfolio Choice with Life Insurance under Uncertainty and Borrowing

Constraints

We develop a duality approach to study a family's optimal consumption, portfolio choice and life insurance purchase when the family receives deterministic labor income which may be terminated due to premature death or retirement of the family's wage earner. The family faces a borrowing constraint and the wage earner has an uncertain lifetime. We establish the existence of an optimal solution to the optimization problem and solve the problem explicitly for several cases.

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CP12

Optimal Dividend Payments for the Piecewise-Deterministic Compound Poisson Risk Model

This work deals with optimal dividend payment problem for a piecewise-deterministic compound Poisson insurance risk model. The objective is to maximize the expected discounted dividend payout up to ruin time. When the dividend payment rate is restricted, the value function is shown to be a solution of the corresponding HJB equation. For the case of unrestricted payment rate, the value function and an optimal barrier strategy are determined explicitly with exponential claim size distributions.

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CP13

On the Credit Risk of Secured Loans

We use stochastic control techniques to analyze the credit risk of secured revolving loans, whose collateral cannot be liquidated immediately. The objective function is a trade-off between the expected loss due to a liquidation event and the shortfall due to the borrower drawing on the credit line less than the full amount available. We exhibit the lender's optimal strategies and compare them with the standard LTV-based lending policy favored by practitioners.

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CP13

Conditional Expected Default Rate Calculations for Credit Risk Applications

Calculation of portfolio loss distributions for large numbers of correlated losses (e.g. credit risk applications) typically use brute force Monte Carlo simulation. We use an asymptotic probabilistic model based on the Central Limit Theorem for solving the portfolio risk aggregation problem for credit risky portfolios. We then prove a theorem that enables efficient computation of the conditional expectation of the default rate for any subportfolio, conditioned on the total portfolio loss. This theorem enables us to solve the capital allocation problem (using expected shortfall as the risk measure) without resorting to Monte Carlo simulation. The approach is very efficient, even for portfolios with several million positions.

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CP13

Measure Changes for Reduced-Form Affine Credit Risk Models

We consider a reduced-form credit risk model, with default intensity driven by an affine process. We fully characterize the family of all locally equivalent probability measures which preserve the structure of the model, providing necessary and sufficient conditions on their density process. In particular, this allows for a rigorous treatment of diffusive and jump-type risk premia. As an application, we characterize the family of all risk-neutral measures for a jump-to-default Heston model.

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CP13

Killed Brownian Motion with a Prescribed Lifetime Distribution and Models of Default

The inverse first passage time problem asks for some distribution whether there is a barrier such that the first time a Brownian motion crosses the barrier has the given distribution. We consider a 'smoothed' version of this problem in which the first passage time is replaced by the first instant that the time spent below the barrier exceeds an independent exponential random variable. We show that any distribution results from some unique barrier.

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CP13

Analysis of Recovery Rate of Non-Performing Consumer Credit

There have been more studies on recovery rate modeling of bonds than on recovery rate modeling of personal loans and retail credit. Little to no research have been conducted on recovery rates in non-performing retail credit with emphasis on third-party buyers. From an empirical point of view, in order to analyze the recovery rate distributions across the different industries, over nine million defaulted or non-performing consumer credit data provided by a German debt collection company are used. A variety of statistical and data mining methods will be examined with respect to prediction and classification. A two-stage model which first classifies debts as extreme or non-extreme with respect to recovery rate is applied; then, the extreme debts are classified into full payment and non-payment. Moreover, the non-extreme recovery rates are predicted in the entire unit interval [0,1].

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CP13

Maximum Likelihood Estimation for Large Interacting Stochastic Systems

Parameter estimation for a large system is facilitated by use of the asymptotic SPDE to which the system weakly converges. Standard particle filtering methods are often not applicable for parameter estimation of the SPDE. A method of moments reduces the SPDE into an SDE system. We then develop a particle filtering method for the SDE system. Theoretical convergence of the finite system's likelihood to the asymptotic likelihood is discussed. Important credit risk and mortgage applications motivate the method.

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MS1

Price Dynamics in Limit Order Markets: Limit Theorems and Diffusion Approximations

We propose a queueing model for the dynamics of a limit order book in a liquid market where buy and sell orders are submitted at high frequency. We derive a functional central limit theorem for the joint dynamics of the bid and ask queues and show that, when the frequency of order arrivals is large, the intraday dynamics of the limit order book may be approximated by a Markovian jump-diffusion process in the positive outhunt, whose characteristics are explicitly described in terms of the statistical properties of the underlying order flow [Cont Larrard 2011]. This result allows to obtain analytical expressions for the probability of a price increase or the distribution of the duration until the next price move, conditional on the state of the order book and characterize various other quantities as solutions of elliptic PDEs in the positive orthant [Cont Larrard 2012]. Our results allow for a wide range of distributional and dependence assumptions in the orders and apply to a wide class of stochastic models proposed for order book dynamics, including Poisson point processes, self-exciting point processes [Cont, Andersen Vinkovskaya 2011] and models of the ACD-GARCH family.

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MS1

Information and the Value of Guaranteed Trade Execution

In many markets, uncertainty about whether a trade is executed can be removed by paying a price premium. We use financial markets as a particular setting in which to study this trade-off. In particular, we assess the role of information in the choice between certain trade at a price premium in an intermediated market such as a dealer market or a limit order book and contingent trade in a dark pool. Our setting consists of intrinsic traders and speculators, each endowed with heterogeneous fine-grained private information as to an assets value, that endogenously decide between these two venues. We solve for an equilibrium in this setting, and address three main questions: First, we illustrate how the choice between certain and contingent trade depends on information available to an individual agent, as well as the overall distribution of information across all agents. Second, we analyze how the premium for certain trade over contingent trade affects the strategic behavior of traders. Finally, we demonstrate how the option for contingent trade affects the ability of intermediating market makers to set transaction costs to maximize profit.

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MS1

Mean-variance Optimal Adaptive Order Execution and Dawson-Watanabe Superprocesses

It is well-known that the mean-variance optimization of adaptive order execution strategies is not dynamically consistent. By localizing the mean-variance criterion, one is led to the optimization of the mean versus quadratic variation, which is a dynamically consistent stochastic control problem with fuel constraint. We show how this latter

problem can be solved by means of Dawson-Watanabe superprocesses.

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MS1
Optimal Liquidation in a Limit Order Book

We consider an asset liquidation problem at the market microstructure level, conditional on observing the limit order book. The optimization problem is formulated in terms of a sequence of stopping times, at which we submit market sell orders. We describe the shape of the trade and no trade regions for various assumptions on the price process and the latency of the trader. In the empirical section, we show that our optimal policy significantly outperforms a benchmark TWAP algorithm on US treasury bonds. In addition we can efficiently calculate the cost of latency in the trade execution.

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MS2
Pricing a Contingent Claim Liability with Transaction Costs Using Asymptotic Analysis for Optimal Investment

We price a contingent claim liability using the utility indifference argument. We consider an agent, who invests in a stock and a money market account with the goal of maximizing the utility of his investment at the final time T in the presence of a proportional transaction cost in two cases with and without the liability. In both cases, we provide a rigorous derivation of the asymptotic expansion of the value function and obtain a "nearly optimal" strategy. Additionally, we derive the asymptotic price of the contingent claim liability.

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MS2
Shadow Prices and Well Posedness in the Optimal Investment and Consumption Problem with Transaction Costs

We revisit the optimal investment and consumption model of Davis and Norman (1990) and Shreve and Soner (1994), following a shadow-price approach similar to that of Kallsen and Muhle-Karbe (2010). Making use of the completeness of the model without transaction costs, we reformulate and reduce the HJB equation for this singular stochastic control problem to a free-boundary problem for a first-order ODE with an integral constraint. Having shown that the free boundary problem has a twicely differenciable solution, we use it to construct the solution of the original optimal investment/consumption problem without any recourse to the dynamic programming principle. Furthermore, we provide an explicit characterization of model parameters for which the value function is finite.

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MS2
Optimal Investment with Small Transaction Costs and General Stochastic Opportunity Sets

For an investor with constant absolute risk aversion, we informally derive the first-order asymptotics of the optimal investment strategy as the bid-ask spread becomes small. For general Itô processes, the first order correction term is expressed in terms of the quadratic variation of the frictionless optimizer. This result allows to quantify the impact of, e.g., predictability and stochastic volatility on portfolio choice in the presence of transaction costs. Applied to an investor holding a random endowment, it also leads to a generalization of the asymptotic utility-based hedging strategies determined by Whalley and Wilmott (1997) for a constant opportunity set. This is joint work with Jan Kallsen.

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MS2
The Optimal Use of Options to Reduce the Effect of Transaction Costs in a Portfolio

Options are redundant in a portfolio of cash and stock if we assume the market of Black and Scholes, which includes no transaction costs. When we include transaction costs, however, options, when used correctly, can become quite useful in reducing the ill-effects these costs create. Specifically, let ε represent the scale of a small proportional loss from any trade. Given an investor's utility preference, the loss in expected utility due to transaction costs in a cash and stock portfolio is, at best, $O\left(\varepsilon^{\frac{2}{3}}\right)$. However, by including options in the portfolio, we can improve this to $O\left(\varepsilon^{\frac{6}{7}}\right)$, which is much closer to the $O(\varepsilon)$ loss guaranteed by even one trade. We detail the specific optimal strategy that accomplishes this.

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MS3

Modeling and Simulation of Systemic Risk in Insurance-Reinsurance Networks

We propose a dynamic insurance network model that allows to deal with reinsurance counter-party default risks with a particular aim of capturing cascading effects at the time of defaults.An equilibrium allocation of settlements is found as the unique optimal solution of a linear programming problem. This equilibrium allocation recognizes 1) the correlation among the risk factors, which are assumed to be heavy-tailed, 2) the contractual obligations, which are assumed to follow popular contracts in the insurance industry (such as stop-loss and retro-cesion), and 3) the interconnections of the insurance-reinsurance network. We are able to obtain an asymptotic description of the most likely ways in which the default of a specific group of insurers can occur, by means of solving a multidimensional Knapsack integer programming problem. Finally, we propose a class of provably strongly efficient estimators for computing the expected loss of the network conditioning the failure of a specific set of companies.

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MS3

Pricing of Path-Dependent Vulnerable Claims in Regime Switching Markets

We study pricing of path-dependent vulnerable claims in regime-switching markets. The key theoretical tool underlying our results is a Poisson series representation of vulnerable claims, which we develop using a change of probability measure technique. We employ such a representation, along with a short-time asymptotic expansion of the claim's price in terms of the Laplace transforms of the symmetric Dirichlet distribution, to develop an efficient method for pricing claims which may depend on the full path of the underlying Markov chain. The proposed approach is applied to price not only simple European claims such as defaultable bonds, but also a new type of path-dependent claims that we term self-decomposable, as well as the important class of vulnerable call and put options on a stock. We provide a detailed error analysis and illustrate the accuracy and computational complexity of our algorithms on market traded instruments, such as defaultable bond prices, barrier options, and vulnerable European options.

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MS3

Default and Systemic Risk in Equilibrium

In a finite horizon continuous time market model, we consider risk averse utility maximizers who invest dynamically in a risk-free money market account, a stock written on a default-free dividend process, and a defaultable bond. Prices are determined via equilibrium. We analyze contagion arising endogenously between the stock and the defaultable bond via the interplay between equilibrium behavior of investors, risk preferences, and cyclicality properties of the default intensity. The equilibrium price of the stock experiences a jump at default, despite that the default event has no causal impact on the dividend process. We characterize the direction of the jump in terms of a relation between investor preferences and the cyclicality properties of the default intensity. A similar analysis is performed for the market price of risk and investor wealth processes. The impact of heterogeneity of preferences on the default exposure carried by different investors is also investigated.

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MS3

Filtered Likelihood for Point Processes

We develop likelihood estimators of the parameters of a marked point process and of incompletely observed explanatory factors that influence the arrival intensity along with the point process itself. The factors follow jump-diffusions whose drift, diffusion, and jump coefficients are allowed to depend on the point process. We provide conditions guaranteeing consistency and asymptotic normality as the sample period grows. We also establish an approximation to the likelihood and analyze the convergence and asymptotic properties of the associated estimators. Numerical results illustrate our approach.

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MS4

Excursions in Atlas Models of Equity Market

Let us consider an equity market of finite number of stocks where behavior of their capitalization is a multidimensional diffusion characterized with their rankings. Such model can capture flows of market capitalizations as it was observed by Fernholz et al. In this talk we consider some questions on excursion measure and time-reversibility for these flows of market capitalization with application to portfolio management under such abstract equity market.

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MS4

Optimal Investment for All Time Horizons and Martin Boundary of Space-time Diffusion

I review the definition and basic properties of the forward performance processes, including their relation to the more standard investment criteria, and the associated SPDE characterization. I, then, concentrate on the problem of constructing the forward investment performance processes in a Markovian setting. In this case, the problem reduces to the so-called "forward Hamilton-Jacobi-Bellman equation", which, in some cases, can be transformed into a time-reversed linear parabolic equation. I characterize the solutions of this (ill-posed) problem explicitly, extending the classical Widders theorem on positive solutions to the time-reversed heat equation. Finally, I consider closed-form examples of the Markovian forward performance processes in some specific stochastic volatility models, including the mean-reverting log-price (Schwartz) model.

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MS4

Volatility-Stabilized Markets

We consider models which generalize the Volatility-stabilized markets introduced in Fernholz and Karatzas (2005). We show how to construct a weak solution of the underlying system of stochastic differential equations, express the solution in terms of time changed squared-Bessel processes, and argue that this solution is unique in distribution. Moreover, we discuss sufficient conditions for the existence of a strong solution and show that strong relative arbitrage opportunities exist in these markets.

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MS4

Generalizations of Functionally Generated Portfolios

I will present generalizations on functionally generated portfolios (FGPs) of stochastic portfolio theory. The assets and the benchmark may be any strictly positive wealth processes, as opposed to merely the stocks and the market portfolio, respectively. Another generalization is that the generating function may be stochastic, so that the generated portfolio can be adjusted to changing market conditions. These FGPs can be applied to arbitrary cointegrated market modes exploiting their mean-reversion in a risk-controlled manner.

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MS5

Optimal Investment in the Presence of High-water Mark Fees

In this talk, we consider the Merton problem for an agent who may invest in a money market fund, a stock, and a hedge fund that is subject to a performance fee. This fee is assessed each time the cumulative profit-to-date derived from the investment in the hedge fund reaches a new running maximum. We will study the associated HJB equation and examine some qualitative properties of the optimal strategy.

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MS5

A Uniqueness Theorem for a Degenerate QVI Appearing in An Option Pricing Problem

We prove the missing uniqueness theorem for the viscosity solution of a degenerate quasi-variational inequality, which makes the probability-free theory of option pricing in the interval market model, essentially complete.

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MS5

Existence, Uniqueness, and Global Regularity for Degenerate Obstacle Problems in Mathematical Finance

The Heston stochastic volatility process, which is widely used as an asset price model in mathematical finance, is a paradigm for a degenerate diffusion process where the degeneracy in the diffusion coefficient is proportional to the square root of the distance to the boundary of the half-plane. The generator of this process with killing, called the elliptic Heston operator, is a second-order degenerate elliptic partial differential operator whose coefficients have linear growth in the spatial variables and where the degeneracy in the operator symbol is proportional to the distance to the boundary of the half-plane. With the aid of weighted Sobolev spaces, we prove existence, uniqueness, and global regularity of solutions to stationary variational inequalities and obstacle problems for the elliptic Heston operator on unbounded subdomains of the half-plane. In mathematical finance, solutions to obstacle problems for the elliptic Heston operator correspond to value functions for perpetual American-style options on the underlying asset.

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MS5

Approximate Solutions to Second Order Parabolic Equations with Time-dependent Coefficients

We consider second order parabolic equations with coefficients that vary both in space and in time (non-autonomous). We derive closed-form approximations to the associated fundamental solution by extending the Dyson-Taylor commutator method that we recently established for autonomous equations. We establish error bounds in Sobolev spaces and show that by including enough terms, our approximation can be proven to be accurate to arbitrary high order in the short-time limit. We show how our method extends to give an approximation of the solution for any fixed time and within any given tolerance. Some applications to option pricing are presented. In particular, we perform several numerical tests, and specifically include results on Stochastic Volatility models.

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MS6

Mixed Deterministic Monte-Carlo Simulations for Finance

Mixing Monte-Carlo and PDE methods can substantially speed-up computations because it allows use of closed form solutions for some of the components. It can also solve problems like unknown boundary conditions for complex stochastic volatility models. Applying the method combined with Longstaff-Schwartz projection can lead to efficient computations of early exercise contracts. The convergence of the methods will be established with error estimates and we shall report performance on multi-dimensional problems.

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MS6

Two-dimensional Fourier Cosine Series Expansion Method for Pricing Financial Options

The COS method for pricing European and Bermudan options with one underlying asset was developed by Fang and Oosterlee (2008, 2009). We extend the method to higher dimensions, with a multi-dimensional asset price process. The algorithm can be applied to, for example, pricing two-color rainbow options, but also to pricing under the Heston stochastic volatility model. For smooth density functions, the method converges exponentially in the number of terms in the Fourier cosine series summations.

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MS6

Risk-Neutral Valuation of Real Estate Options

We propose a novel and intuitive risk-neutral valuation model for real estate derivatives. The resulting index behavior can easily be analyzed and closed-form pricing solutions are derived for forwards, swaps and European put and call options. We demonstrate the application of the model by valuing a put option on a house price index. Autocorrelation in the index returns appears to have a large impact on the option value. We also study the effect of an over- or undervalued real estate market. The observed effects are significant and as expected.

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MS6

Efficient Option Pricing of Asian Options based on Fourier Cosine Expansions

In this talk we present an efficient pricing method for Asian options under Lévy processes, based on Fourier–cosine expansions and Clenshaw–Curtis quadrature. The pricing method has been developed for both European–style and American–style Asian options, written on different types of average (arithmetic, geometric and harmonic), and for discretely and continuously monitored versions. Fast convergence of Fourier cosine expansions and Clenshaw–Curtis quadrature ensures exponential convergence in the Asian option prices in most cases, which reduces the computing time of the method to milliseconds for geometric Asian options and a few seconds for arithmetic Asian options. The method's convergence behavior is explained by an error analysis. Its performance is further demonstrated by various numerical examples, where we also show the power of an implementation on the Graphics Processing Unit (GPU) where hundreds of speedup is achieved for pricing early–exercise Asian options, in particular.

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MS7

Sampling Error of the Supremum of a Levy Process

Lvy processes are often used in finance to model the dynamics of asset prices. The supremum of a Lvy process is of interest when one is pricing financial contracts whose payoffs depend on the supremum of the underlying asset price process. While the maximum of a discretely sampled Lvy process can often be handled very efficiently using numerical methods, not much is known about the continuous supremum of a general Lvy process. We present results on the discrepancy between the discrete maximum and continuous supremum of a Lvy process. Using Spitzers identity and results from analytic number theory, we derive explicit expressions for the sampling errors for various commonly used Lvy processes. The results help us better understand the error of approximating the continuous supremum of a Lvy process by a discrete maximum.

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MS7

Positive Subordinate CIR Processes with Two-Sided Mean-Reverting Jumps

We present the SubCIR jump-diffusion process. The SubCIRsdiffusion dynamics are those of a CIR process. The SubCIRs jump componentincludes two-sided mean-reverting (state-dependent) jumps. The process remainsstrictly positive if the CIR process satisfies Fellers condition. Theanalytical tractability of the SubCIR process makes it a richer extension tothe CIR process (compared to previous models) and it is also a naturalalternative for interest rates and credit models.

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MS7

Default Swap Games

We consider the valuation of game-type credit default swaps that allow the protection buyer and seller to raise or reduce the respective position once prior to default. Under a structural credit risk model based on spectrally negative Levy processes, we analyze the existence of the Nash equilibrium and derive the associated saddle point. Using the principles of smooth and continuous fit, we determine the buyer's and seller's equilibrium exercise strategies, which are of threshold type.

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MS7

Multifactor Term Structure of Interest Rates under Regime Shifts and Levy Jumps

We develop a tractable dynamic term structure models under jump-diffusion with Levy Jumps and regime shifts with time varying transition probabilities. The model allows for regime-dependent jumps while both jump risk and regime-switching risk are priced. Two types solutions, including (log-linear) approximate solutions and exact solutions for the term structure are obtained for affine-type models under different conditions. For the approximate solutions, we derive the error bound, which is in the first order only. For the exact solutions, we further obtain closed-form expressions for special cases. Joint work with Xiangdong Liu, Lawrence C. Evans, and Shu Wu.

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MS8

Risk Measures and Fine Tuning of High Frequency Trading Strategies

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MS8

New Models for Optimal Execution and High-frequency Market Making

Two related papers will be presented that rely on the same mathematical finding. The first one "Dealing with the inventory risk" solves the Avellaneda-Stoikov problem. It corresponds to the case of a market maker who has to continuously set a bid and a ask quote and we derive the optimal quotes with closed-form approximations based on spectral ideas. The second one deals with the classical subject of optimal liquidation and is one of the first attempts to solve the problem with limit orders instead of liquidity-consuming market orders. This second paper will be presented for very general intensity functions.

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MS8

Optimal HF Trading in a Prorata Microstructure

We propose a framework to study optimal trading policies in a one-tick pro-rata limit order book, as typically arises in short-term interest rate futures contracts. The high-frequency trader has the choice to trade via market orders or limit orders, which are represented respectively by impulse controls and continuous controls. We model and discuss the consequences of the two main features of this particular microstructure: first, the limit orders sent by the high frequency trader are only partially executed, and therefore she has no control on the executed quantity. For this purpose, cumulative executed volumes are modelled by compound Poisson processes. Second, the high frequency trader faces the overtrading risk, which is the risk of brutal variations in her inventory. The consequences of this risk are investigated in the context of optimal liquidation. The optimal trading problem is studied by stochastic control and dynamic programming methods, which lead to a characterization of the value function in terms of an integro quasi-variational inequality. We then provide the associated numerical resolution procedure, and convergence of this computational scheme is proved. Next, we examine several situations where we can one one hand simplify the numerical procedure by reducing the number of state variables, and on the other hand focus on specific cases of practical interest. We examine both a market making problem and a best execution problem in the case where the mid-price process is a martingale. We also detail a high frequency trading strategy in the case where a (predictive) directional information on the mid-price is available. Each of the resulting strategies are illustrated by numerical tests.

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MS9

Stochastic Perron's Method and Verification without Smoothness using Viscosity Comparison: Obstacle Problems and Dynkin Games

We adapt the Stochastic Perron's method in Bayraktar and Sirbu (to appear in the Proceedings of the American Mathematical Society) to the case of double obstacle problems associated to Dynkin games. We construct, symmetrically, a viscosity sub-solution which dominates the upper value of the game and a viscosity super-solution lying below the lower value of the game. If the double obstacle problem satisfies the viscosity comparison property, then the game has a value which is equal to the unique and continuous viscosity solution. In addition, the optimal strategies of the two players are equal to the first hitting times of the two stopping regions, as expected. The (single) obstacle problem associated to optimal stopping can be viewed as a very particular case. This is the first instance of a non-linear problem where the Stochastic Perron's method can be applied successfully. (Joint work with Mihai Sirbu. Available on ArXiv.)

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MS9

Optimal Consumption and Investment in Incomplete Markets with General Constraints

We study an optimal consumption and investment problem in a possibly incomplete market with general, not necessarily convex, stochastic constraints. We give explicit solutions for investors with exponential, logarithmic and power utility. Our approach is based on martingale methods which rely on recent results on the existence and uniqueness of solutions to BSDEs with drivers of quadratic growth.

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MS9

Dynamic Portfolio Choice with Multiple Decentralized Agents

Abstract not available at time of publication.

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MS9

Constructing Sublinear Expectations on Path Space

We provide a general construction of time-consistent sublinear expectations on the space of continuous paths. It yields the existence of the conditional G-expectation of a Borel-measurable (rather than quasi-continuous) random variable, a generalization of the random G-expectation, and an optional sampling theorem that holds without exceptional set.

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MS10

Resilience to Contagion in Financial Networks

Propagation of balance-sheet or cash-flow insolvency across financial institutions may be modeled as a cascade process on a network representing their mutual exposures. We derive rigorous asymptotic results for the magnitude of contagion in a large financial network and give an analytical expression for the asymptotic fraction of defaults, in terms of network characteristics. Our results extend previous studies on contagion in random graphs to inhomogeneous directed graphs with a given degree sequence and arbitrary distribution of weights. We introduce a criterion for the resilience of a large financial network to the insolvency of a small group of financial institutions and quantify how contagion amplifies small shocks to the network. Our results emphasize the role played by "contagious links' and show that institutions which contribute most to network instability in case of default have both large connectivity and a large fraction of contagious links. The asymptotic results show good agreement with simulations for networks with realistic sizes.

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MS10

Coupled Diffusions, Swarming and Systemic Risk

Abstract not available at time of publication.

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MS10

Failure and Rescue in an Interbank Network

This paper is concerned with systemic risk in the interbank market. We model this market as a directed graph in which the banks represent the nodes and the liabilities between the banks represent the edges. Our work builds on the modelling paradigm of Eisenberg and Noe (2001), extending it by introducing default costs in the system. We provide a rigorous analysis of those situations in which banks have incentives to bailout distressed banks. Such incentives exist under very mild conditions. We illustrate our results with some simple examples, and go on to discuss possible measures of soundness of a financial system, together with possible policy implications for resolution of distress.

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MS10

Feedback Effects and Endogenous Risk in Financial Markets

We present a mathematical model which allows to quantify the impact of fire sales of assets of a fund undergoing losses on the volatilities and correlations of assets held by the fund. Our model shows that the liquidation of large positions by funds may result in spikes in volatilities and correlations, even in absence of liquidity dry-up, and gives plausible explanations for the large hedge fund losses of August 2007. We show that our model can be used for forensic analysis of financial data, to recover characteristics of the portfolio undergoing fire sales from public data, by solving an inverse problem. We show the consistency of the estimator obtained and apply it to simulated and empirical data.

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MS11

Dynamic Modeling of Systemic Risk

We generalize the Eisenberg-Noe model to allow for multiple clearing dates, as well as uncertainty in future liabilities and cash inflows. The clearing payment vectors are sequentially recovered as the solutions of robust linear programming problems solved over the planned horizon. We show existence and uniqueness of the clearing payment vectors over time. We perform a sensitivity analysis of the loss and payment vector with respect to borrowing and equity constraints. We employ the Shapley value methodology to dynamically attribute the systemic risk to the individual nodes in the network. We conclude with a numerical assessment of the proposed methodology on a systemic network consisting of a large number of highly interconnected financial institutions.

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MS11

Estimating Hedge Fund Risk Factors

The estimation of hedge fund returns and the risk factors that impact them is a critical step in the construction of portfolios. In particular, so called fund-of-funds have the arduous task of building portfolios of hedge fund strategies based on limited and low frequency observations. This is quite daunting in the hedge fund space due to the generally small sample sizes and opaque nature of that industry's data. To overcome these difficulties, it is desired to estimate risk factors based on market observables and reverse engineer a hedge fund exposure to those factors. The model that we propose will be used to analyze and decompose the risk of various hedge fund indices on common factors at a high frequency (e.g., daily, or intra-day) based on their habitual low frequency observations (typically monthly). Specifically, we will jointly model the risk-factors (e.g., stock returns) and the asset returns (e.g., a hedge fund strategy) in a fat-tailed, stochastic volatility environment implemented with a Bayesian approach via a Rao-Blackwellised (R-B) particle filter. We utilize a vector Stochastic-Volatility model with smoothed observable returns to extract the potentially time-varying exposure of low frequency hedge fund performance on high frequency data. By making use of a particle filter with Rao-Blackwellization, we reduce the parameter space significantly resulting in a more accurate estimate of the distibution of the parameter state. This approach can be used for analyzing hedge fund performance and their advertized strategies as well as in forensic risk-management. The latter of which is a critical need given the generally

low transparency of the hedge fund industry.

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MS11

Smooth and Monotone Covariance Estimation for Elliptical and Generalized Hyperbolic Distributions

We consider the problem of high-dimensional covariance estimation from severely limited observations. Strong assumptions on the structure of the underlying random vector have to be made for the problem to be well-defined. Some examples developed in the literature include: covariance selection models with sparse inverse covariances, low-rank structures (PCA models and factor analysis), sparse plus low-rank structures, multi-scale structures. We consider another assumption which is important for a variety of applications including term-rate risk-modeling in computational finance: smoothness and monotonicity. We review our previous formulation for multivariate Gaussian random vectors based on semi-definite programming, and extend the method for elliptical and generalized hyperbolic distributions. We use efficient convex optimization algorithms and compare the methods using various penalized Bregman divergences as objective functions with examples from interest rate modeling.

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MS11

Nonparametric Prediction in a Limit Order Book

We propose a novel non-parametric approach to short-term forecasting of the mid-price in a limit order book. We introduce a state vector describing the state of the order book at each time. The predictor is based on two features, computed for each value of the state vector. Implicit assumptions of our method are very mild and are supported by our preliminary real-data experiments on NYSEs OpenBook which yield promising empirical results.

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MS12

Dynamic Assessment Indices

Measuring performance and risk of cash flows is a crucial issue in finance. A Dynamic Assessment Index (DAI) is a quasiconcave, monotone function, mapping cash flows into processes which represent their risk or performance evaluations in time. Using L^0-separation theorems, we provide an upper semicontinuous robust representation and study the impact of different time consistency conditions; in particular, how past performances may impact the present assessment of risk. Illustrative examples will be discussed.

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MS12

Minimal Supersolutions of BSDEs and Robust Hedging

We study minimal supersolutions of BSDEs - related to Peng's g-expectation - which can be seen as superhedging functionals. We prove existence, uniqueness, monotone convergence, Fatou's Lemma and lower semicontinuity of our functional. Unlike usual BSDE methods, based on fixed point theorems, the existence relies on compactness methods. We then study some robust extensions which correspond to the problem of superhedging under volatility uncertainty. The talk is based on joint works with Samuel Drapeau and Gregor Heyne.

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MS12

Set-valued Dynamic Risk Measures in Markets with Transaction Costs

Set-valued risk measures appear naturally when markets with transaction costs are considered and capital requirements can be made in a basket of currencies or assets. In this talk we study dual representation and time consistency properties of dynamic set-valued risk measures. It turns out that only a stronger time consistency called multi-portfolio time consistency is equivalent to a recursive form of the risk measure as well as to an additive property for the acceptance sets, which is a central result in the scalar case.

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MS12

Portfolio Choice with Time-consistent Dynamic Risk Measures

We study portfolio selection based on time-consistent dynamic risk measures in a general continuous-time setting. The setting features discontinuities in the asset price processes, with a general and possibly infinite activity jump part besides a continuous diffusion part, and general and possibly non-convex trading constraints. We characterize the minimal risk processes as solutions to Backward Stochastic Differential Equations (BSDEs). We prove existence and uniqueness of the solution in the general class of jump BSDEs having a driver function that grows at most quadratically. We further compute these solutions in a few examples by numerically solving the corresponding BSDEs using regression techniques.

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MS13

The Valuation of Double Barrier Options under Multifactor Pricing Models

The (vast) literature on the pricing of barrier options is mainly focused on the valuation of European-style contracts under single-factor option pricing models (such as the geometric Brownian motion and the CEV processes). This paper extends the literature in two directions. First, European-style (double) barrier options are priced under a multifactor and Markovian financial model that is able to accommodate stochastic volatility, stochastic interest rates, endogenous bankruptcy, and time-dependent barriers. Second and more importantly, quasi-analytical pricing solutions are also proposed for American-style (double) barrier option contracts under the same general financial model. The proposed pricing solutions are shown to be accurate, easy to implement, and efficient.

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MS13

Exponential Time Differencing Methods for Pricing and Hedging American Options

Exponential time differencing (ETD) methods based on the Cox and Matthews approach are developed to solve a nonlinear BlackScholes model for pricing and hedging American options with transaction cost. Each of these methods avoids solving nonlinear systems, whilst, well known standard methods would require solving nonlinear systems at each time step. Numerical experiments are performed on exotic path-dependent American options with transaction cost to demonstrate the computational efficiency, accuracy and reliability of the methods.

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MS13

Efficient and Robust Time Stepping Under Jump-diffusion Models

Partial-integro differential (PIDE) formulations are often used to solve option pricing problems where the underlying asset follows a jump-diffusion process. The main challenge lies in the efficient treatment of the jump term resulting a full matrix. We discuss some efficient, robust, and accurate time discretization methods including schemes treating the jump term explicitly.

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MS13

Pricing American Options Under Jump-diffusion Models

Under jump-diffusion models, a linear complementarity problem (LCP) with a partial-integro differential operator can formulated for the price of an American option. As the discretization of the jump term leads to a full matrix, it preferable to use special techniques to solve the resulting LCPs. We discuss various efficient methods for these LCPs.

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MS14

Efficient Laplace Inversion, Wiener-Hopf Factorization and Pricing Lookbacks

We construct very fast and accurate methods of approximate Laplace inversion, calculation of the Wiener-Hopf factors for wide classes of Levy processes with exponentially decaying Levy densities, and pricing lookback options. In all cases, we use appropriate conformal changes of variables, which allow us to apply the simplified trapezoid rule with small number of terms. The same technique is applicable for calculation of pdf's of the supremum and infimum processes, and prices and sensitivities of options with lookback and barrier features.

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MS14

Quadratic Hedging of Barrier Options under Leptokurtic Returns Driven by an Exponential Lvy Model

We examine quadratic hedging of barrier options in a model realistically calibrated to reflect the leptokurtic nature of equity returns. We compute the hedging error of the optimal hedging strategy andevaluate prices that yield reasonable risk-adjusted performance for the hedger. Our main finding is that the impact of hedging errors on prices is several times higher than the impact of other pricing biases studied in the literature, in particular the effect of barrier misalignment and of discrete monitoring.

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MS14

Exact Simulation of the Heston Jump-Diffusion

In this talk, we extend the Heston stochastic volatility model to include state-dependent jumps in the price and the volatility, and develop a method for the exact simulation of this model. The jumps arrive with a stochastic intensity that may depend on time, price, volatility and jump counts. They may have an impact on the price or the volatility, or both. The random jump size may depend on the price and volatility. Numerical experiments illustrate the features of the exact method. This is a joint work with Prof. Erhan Bayraktar at the University of Michigan and Prof. Kay Giesecke at Stanford University.

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MS14

Efficient Pricing and Reliable Calibration in the Heston Model and its Generalizations

We suggest a general scheme for improvement of FT-pricing formulas for European option and give efficient recommendations for the choice of the parameters of the numerical scheme, which allow for very accurate and fast calculations. We demonstrate that an indiscriminate choice of parameters of a numerical scheme leads to an inaccurate pricing and calibration. As applications, we consider the Heston model and its generalization, and several other affine models. For many parameter sets documented in empirical studies of financial markets, relative accuracy better than 0.01 % can be achieved by summation of less than 10-20 terms even in the situations in which the standard approach requires more than 200. In some cases, the one-term formula produces an error of several percent, and the summation of two terms — less than 0.5 %. Typically, 10 terms and fewer suffice to achieve the error tolerance of several percent and smaller.high-level commands.

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MS15

Central Clearing Mechanisms for Credit Default Swaps

Central clearing of Credit default swaps through Central Counterparties (CCPs) has been proposed as a tool for mitigating systemic risk and counterpart risk in CDS markets. The design of CCPs for CDS involves the implementation of margin requirements and a clearing fund (or default fund), for which various designs have been proposed. We study the impact of the design of these requirements on the risk of the CCP and the incentives for CDS clearing.

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MS15

Central Clearing of OTC Derivatives : Bilateral vs Multilateral Netting

We study the impact of a central counterparty (CCP) for OTC derivatives on expected interdealer exposures. The results are sensitive to assumptions on heterogeneity of risk across asset classes as well as correlation of exposures across asset classes; empirically plausible specifications of these parameters lead to the conclusion that the gain from multilateral netting in a CCP largely overweighs the loss of netting across asset classes in bilateral netting agreements.

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MS15

Measuring Contagion in Financial Networks

Liabilities between financial entities form a network. The clearing of liabilities and thereby contagion of risk and default depend on this network structure. We provide a mathematical model to understand clearing and propagation of default in such financial networks. This yields a precise measure for the systemic risk induced by individual financial entities. The model allows to compute optimal bailout strategies that either minimize the cost of the intervention or maximize the stabilizing effect for a given bailout budget. Finally, the computational efficiency of the model allows to analyze large scale networks quickly.

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MS15

Are CDS Auctions Biased?

We study settlement auctions for credit default swaps (CDS). We find that the one-sided design of CDS auctions used in practice gives CDS buyers and sellers strong incentives to distort the final auction price, in order to maximize payoffs from existing CDS positions. Consequently, these auctions tend to overprice defaulted bonds conditional on an excess supply and underprice defaulted bonds conditional on an excess demand. We propose a double auction to mitigate this price bias. We find the predictions of our model on bidding behavior to be consistent with data on CDS auctions.

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MS16

Endogenous Equilibria in Liquid Markets with Frictions and Boundedly Rational Agents

We propose a simple binary mean field game, where N boundedly rational agents may decide to trade or not a share of a risky asset in a liquid market. Agents' utility depends on returns, which are endogenously determined taking into account observed and forecasted demand and an exogenous transaction cost. The explicit dependence on past demand generates endogenous dynamics of the system. It is shown that pure strategy Nash equilibria exist. We study under a rather general setting (risk attitudes, pricing rules and noises) the aggregate demand for the asset, the emerging returns and the structure of the equilibria of the asymptotic game. We prove that boom and crash cycles may arise and that transaction costs have a stabilizing effect on the market.

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MS16

Large Portfolio Asymptotics for Loss From Default

We prove a law of large numbers for the loss from default and use it for approximating the distribution of the loss from default in large, potentially heterogenous portfolios. The density of the limiting measure is shown to solve a non-linear SPDE, and the moments of the limiting measure are shown to satisfy an infinite system of SDEs. The solution to this system leads to the distribution of the limiting portfolio loss, which we propose as an approximation to the loss distribution for a large portfolio. Numerical tests illustrate the accuracy of the approximation, and highlight its computational advantages over a direct Monte Carlo simulation of the original stochastic system.

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MS16

Branching and Interacting Particle Models of Systemic Risk

We propose an interacting particle system description of the banking system. While net bank assets evolve independently under normal conditions, defaults trigger a mean-field type interaction that creates systemic risk. We work with a stochastic size of the economy, with new banks added spontaneously according to a mean-field birth process. We present some preliminary results about system stability and the properties of the corresponding mean-field limit.

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MS16

Most Likely Path to Systemic Failure

In this talk, I will present recent results on modeling the dynamics of correlated default events in the financial market. An empirically motivated system of interacting point processes is introduced and we study how different types of risk, like contagion and exposure to systematic risk, compete and interact in large-scale systems. Large deviation arguments are used to approximate the tail of the default loss in large portfolios and to identify the way that atypically large (i.e. “rare’) default clusters are most likely to occur. The results give insights into how different sources of default correlation interact to generate atypically large portfolio losses.

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MS17

Quasi-convex Dynamic Programming for Storage Evaluation

The value of a storage facility can often be represented as a quasi-convex function of the market price and current capacity utilization. This talk will describe a dynamic programming procedure to take advantage of this structure. The method relies on progressive refinement of outer approximations of the sub-level sets of the value function in each stage.

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MS17

A Kernel Based Approach to Gas Storage and Swing Contracts Valuations in High Dimensions

We are expanding upon our previous work [Boogert and Mazieres, "A Radial Basis Function Approach to Gas Storage Valuation", 2011], by introducing multi-factor price and volume dimensions encountered in both gas storage and swing contracts. This is achieved by introducing new multivariate methods (Kernel based: Radial Basis Functions and the Tensor of Radial Basis Functions) to the multi-dimensional Least-Squares Monte Carlo method used to value these contracts with the spot approach.

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MS17

Approximate Linear Programming Relaxations for Commodity Storage Real Option Management

The real option management of commodity conversion assets based on high dimensional forward curve evolution models commonly used in practice gives rise to intractable Markov decision processes. Focusing on commodity storage, we derive approximate dynamic programs from relaxations of approximate linear programs formulated using low dimensional value function approximations. We evaluate the performance of our approximate dynamic programs on natural gas and oil instances.

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MS17

Natural Gas Storage Valuation, Optimization, Market and Credit Risk Management

We present a model for the valuation, optimization, and pricing of the credit risk of gas storage contracts. A reduced form term structure model of the curve dynamics is derived that facilitates dimension reduction without sacrificing realism. A system of PDEs is derived and solved using RBF collocation. When the number of injection/withdrawal opportunities is large, RBF-PDE method can solve problems where heuristic approaches would be impractical. The RBF expansions facilitate pricing of credit risk.

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MS18

Small-time Expansions for Stochastic Volatility Models with Lévy Jumps

We analyze the short-time (equivalently, near expiration) behavior of the tail distributions and option prices of a class of stochastic volatility (SV) models obtained by superposing a classical continuous SV process (say, the Heston process) with an independent pure-jump Lévy process. Polynomial expansions in time of arbitrary order are obtained for the tail distributions and out-of-the money option prices, assuming certain smoothness conditions on the Lévy density of the jump component and a small-time large deviation principle for the continuous component. As a result, we are able to disentangle the effects of the various model parameters in the short-time behavior of the option prices and rank their contribution according to the first power at which they appear in the polynomial expansion. This talk is based on a joint work with C. Houdré and R. Gong.

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MS18

Large Deviations and Stochastic Volatility with Jumps: Asymptotic Implied Volatility for Affine Models

We consider the implied volatility of European options in an affine stochastic volatility model with jumps, as time tends to infinity. We show that under a simultaneous rescaling of the option strike a non-degenerate limiting volatility smile exists and describe it by a formula which can be expressed in terms of the parameters of the underlying model. The result is based on a large-deviation principle for affine stochastic volatility models, that is derived via the Gärtner-Ellis theorem. We exhibit some specific examples including a Heston model with and without jumps, Bates' model with state-dependent jump intensity and the Barndorff-Nielsen-Shephard model.

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MS18

A New Look at Short-term Implied Volatility in Models with Jumps

This talk analyses the behaviour of the implied volatility smile for short-dated options in semimartingale models with jumps. We introduce a new renormalization of the strike variable such that the implied volatility for short-maturity options converges to a nonconstant finite limit, characterised by the diffusion and jump components of the model. This limit yields calibration algorithms for short-dated options and sheds new light on the difference between finite and infinite variation jumps in pricing models.

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MS18

Parametric Inference and Dynamic State Recovery from Option Panels

We develop parametric estimation procedure for option panels observed with error. We provide semiparametric tests for the option price dynamics based on the distance between the spot volatility extracted from the options and the one obtained nonparametrically from high-frequency data on the underlying asset. We further construct new formal tests of the model fit for specific regions of the volatility surface and for the stability of the risk-neutral dynamics over a given period of time.

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MS19

A Decomposition Formula for Option Prices in the Heston Model and Applications to Option Pricing Approximation

By means of classical Its calculus we decompose option prices in the Heston volatility framework as the sum of the classical Black-Scholes formula with volatility parameter equal to the root-mean-square future average volatility plus a term due to correlation and a term due to the volatility of the volatility. This decomposition formula allows us to construct first and second order option pricing approximation formulas that are extremely easy to compute, as well as to study their accuracy for short maturities. Moreover we see the corresponding approximations for the implied volatility are linear (first-order approximation) and quadratic (second-order approximation) in the log-stock price variable.

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MS19

Small-noise Expansion for Projected Diffusions and Implied Volatility Asymptotics

Given a diffusion in R^n, we prove a small-noise expansion for the density of its projection on a subspace of dimension $p \leq n$. Our proof relies on the Laplace method on Wiener space and stochastic Taylor expansions in the spirit of Azencott-Benarous-Bismut. Our result (assuming Hörmander's condition on the vector fields) applies to (i) small-time asymptotics, (ii) tails of the distribution and (iii) small-noise expansions. In the context of stochastic volatility models, we recover the Busca-Berestycki-Florent formula (applying (i)) and Gulisashvili-Stein expansion (from (ii)). This is a joint work with J.D. Deuschel (TU Berlin), P. Friz (TU Berlin) and S. Violante (Imperial College London).

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MS19

Asymptotics of Implied Volatility to Arbitrary Order

In a unified model-free framework that includes long-expiry, short-expiry, extreme-strike, and jointly-varying strike-expiry regimes, we find asymptotic implied volatility and implied variance formulas in terms of L, with rigorous error estimates of order $1/L$ to any given power, where L denotes the absolute log of an option price that approaches zero. Our results therefore sharpen, to arbitrarily high order of accuracy, the model-free asymptotics of implied volatility in extreme regimes. We then apply these general formulas to particular examples: Lévy and Heston. Joint work with Kun Gao.

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MS19

Multi-Factor Stochastic Volatility Models for Options and Options on Variance

Through perturbation methods we reconcile skews of implied volatilities for options and options on variance in the context of multi-scale stochastic volatility models.

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MS20

On the Multi-Dimensional Controller and Stopper Games

We consider a zero-sum stochastic differential controller-and-stopper game in which the state process is a controlled diffusion evolving in a multi-dimensional Euclidean space. In this game, the controller affects both the drift and the volatility terms of the state process. Under appropriate conditions, we show that the game has a value and the value function is the unique viscosity solution to an obstacle problem for a Hamilton-Jacobi-Bellman equation.

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MS20
Numerical Solutions of Optimal Risk Control and Dividend Optimization Policies

This work develops numerical methods for finding optimal dividend pay-out and reinsurance policies. The surplus is modeled by a regime-switching process subject to both regular and singular controls. Markov chain approximation techniques are used to approximate the value function and optimal controls. The proofs of the convergence of the approximation sequence to the surplus process and the value function are given. Examples are presented to illustrate the applicability of the numerical methods.

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MS20
Outperformance Portfolio Optimization via the Equivalence of Pure and and Randomized Hypothesis Testing

We study the portfolio problem of maximizing the outperformance probability over a random benchmark through dynamic trading with a fixed initial capital. Under a general incomplete market framework, this stochastic control problem can be formulated as a composite pure hypothesis testing problem. We analyze the connection between this pure testing problem and its randomized counterpart, and from latter we derive a dual representation for the maximal outperformance probability. Moreover, in a complete market setting, we provide a closed-form solution to the problem of beating a leveraged exchange traded fund. For a general benchmark under an incomplete stochastic factor model, we provide the Hamilton-Jacobi-Bellman PDE characterization for the maximal outperformance probability.

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MS20
Optimal Trend-following Trading Rules under a Three-state Regime-switching Mode

Assume the market follows a regime switching model with three states, a set of sufficient conditions are developed to guarantee the optimality of trend-following trading strategies. A dynamic programming approach is used to verify these optimality conditions. The value functions are characterized by the associated HJB equations. The results in this paper will help an investor to identify market conditions and to avoid trades which might be unprofitable even under the best market information.

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MS21
Evaluating Callable and Putable Bonds: An Eigenfunction Expansion Approach

Abstract not available at time of publication.

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MS21
Building Financial Models with Time Changes

Abstract not available at time of publication.

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MS21
Pricing Derivatives on Multiscale Diffusions: An Eigenfunction Expansion Approach

Using tools from spectral analysis, singular and regular perturbation theory, we develop a systematic method for analytically computing the approximate price of a derivative-asset. The payoff of the derivative-asset may be path-dependent. Additionally, the process underlying the derivative may exhibit killing (i.e. jump to default) as well as combined local/nonlocal stochastic volatility. The nonlocal component of volatility is multiscale, in the sense that it is driven by one fast-varying and one slow-varying factor. The flexibility of our modeling framework is contrasted by the simplicity of our method. We reduce the derivative pricing problem to that of solving a single eigenvalue equation. Once the eigenvalue equation is solved, the approximate price of a derivative can be calculated formulaically. To illustrate our method, we calculate the approximate price of three derivative-assets: a vanilla option on a defaultable stock, a path-dependent option on a non-defaultable stock, and a bond in a short-rate model.

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MS21

Closed-form Expansions of Option Prices under Time-changed Dynamics

We consider a broad class of option pricing models and derive a simple closed-form expansion of option prices in these models in terms of Black-Scholes prices and higher-order Greeks. The expansion provides a transparent and informative decomposition of option prices. Moreover, it can be used for a large class of flexible models which allow for both stochastic volatility and jumps. Finally, it allows for fast model calibration.

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MS22

Optimal Portfolios under Worst Case Scenarios

Standard portfolio theories such as Expected Utility Theory, Yaari's Dual Theory, Cumulative Prospect Theory and Mean-Variance optimization all assume that investors only look at the distributional properties of strategies and do not care about the states of the world in which the cash-flows are received. In a very interesting paper, Dybvig (1988a, 1988b) essentially showed that in these instances optimal portfolios are decreasing in the state-price density, also pointing indirectly to the important role of diversified portfolios. In this paper we first observe that the worst outcomes for optimal strategies exactly occur when the market declines (i.e. during a financial crisis), but this is at odds with the aspirations and requirements of many investors. Hence we depart from the traditional behavioral setting and study optimal strategies for investors who do not only care about the distribution of wealth but, additionally, also impose constraints on its interaction with the (stressed) financial market. Preferences become state-dependent and we are able to assess the impact of these on trading decisions. We construct optimal strategies explicitly and show how they outperform traditional diversification strategies under worst-case scenarios.

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MS22

Myopic Loss Aversion, Reference Point, and Money Illusion

We use the portfolio selection model presented in He and Zhou (2011, *Management Science*, Volume 57, Issue 2, pages 315–331) and the NYSE equity and U.S. treasury bond returns for the period 1926-1990 to provide a rigorous treatment of Benartzi and Thaler's myopic loss aversion theory. We find that in addition to the agent's loss aversion and evaluation period, his reference point also has a significant effect on optimal asset allocation. We demonstrate that the agent's optimal allocation to equities is consistent with the market observation when he has reasonable values of degree of loss aversion, evaluation period, and reference point. We also find that the optimal allocation to equities is sensitive to these parameters. We then examine the implications of money illusion for asset allocation and pricing. Finally, we extend the model to a dynamic setting.

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MS22

Consumption-based Behavioral Portfolio Selection in Continuous Time

We study the optimal consumption-investment problem in a continuous-time financial market with behavioural criteria featured by S-shaped utility function and probability distortions. Different formulations of the problem are studied. When optimal solutions exist, we get explicit forms based on some algebraic equations.

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MS22

Utility Maximization with Addictive Consumption Habit Formation in Incomplete Markets

We study the utility maximization problem of consumption with addictive habit formation in the general incomplete semimartingale market. By introducing the auxiliary state and dual processes and defining the value function both on initial wealth and initial habit, we embed our original path dependent problem into an abstract time separable optimization problem with the shadow random endowment. We establish existence and uniqueness of the optimal solution using convex duality approach on L^0_+ spaces.

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MS23

The Log Optimal Portfolio under Transaction Costs and the Shadow Price: The Geometric Ornstein-Uhlenbeck Process and a Counterexam-

ple

As in (Gerhold/Muhle-Karbe/Schachermayer 2011) we find the growth optimal portfolio for the geometric Ornstein-Uhlenbeck process under proportional transaction costs by constructing a shadow price. This is a price process, such that the optimization problem without frictions for that price has the same solution as the one under transaction costs. This technique allows us to explicitly compute fractional Taylor expansions of arbitrary order for all quantities of interest. Similar results have (to the best of our knowledge) so far only been obtained for the Black Scholes model. Moreover, we present a counterexample that shadow prices may not exist in general even in discrete time and for "well-behaved' markets.

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MS23

Market Depth and Trading Volume Dynamics

We derive the process followed by trading volume, in a market with finite depth and constant investment opportunities. A representative investor, with a long horizon and constant relative risk aversion, trades a safe and a risky asset with a liquidity cost proportional to trading speed. An ordinary differential equation identifies the trading policy and welfare. In the high-liquidity limit, trading volume follows approximately an Ornstein-Uhlenbeck process, and increases with liquidity, volatility, and risk aversion.

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MS23

Long-run Investment under Drawdown Constraints: optimal portfolios and numeraire property

We consider long-run investment problems under drawdown constraints: the current wealth can not fall below a given function of its past maximum. We work in a general semimartingale setting. First, we show that this problem is equivalent to an unconstrained problem but with a modified utility function: both the value and the optimal portfolio are given explicitly in terms of their unconstrained counterparts (joint work with Vladimir Cherny). Second, we analyse in more detail the growth optimal portoflio under linear drawdowns. We show it enjoys the numeraire property along specific sequences of stopping times and asymptotically but not for all times. A turnpike theorem shows it is a limit of numeraire strategies on finite horizons (joint work with Constantinos Kardaras and Eckhard Platen).

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MS23

Wealth vs Risk in a Continuous Time Model

We discuss a continuous time optimization problem which combines two conflicting objectives of maximizing the portfolio wealth up to a level and minimizing the conditional value-at-risk of the portfolio wealth loss. The associated utility function is not differentiable nor strictly concave and does not satisfy Inada's condition. We use the dual control method to show that there is a classical solution to the HJB equation and that the optimal value function is smooth if the optimal control satisfies an exponential moment condition. We find the closed-form optimal feedback control and optimal value function for a wealth maximization problem.

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MS24

Stress Tests: From Arts to Science (Overview)

Expectations on stress tests are high in the financial industry: they should measure the resilience of individual financial institutions and of the whole banking system as part of an economy. Additionally, they should act as a calmative for nervous markets. It is time to assess the expectations about what information can realistically be obtained from stress tests. How should we choose scenarios which are at the same time plausible and informative of potential weaknesses? How can we assess the validity of our models and the potential consequences where our models break down? How can we adequately discriminate adverse external shocks and dangerous endogenous effects?

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MS24

Finding Stress Scenarios That Get the Job Done, with Credit Risk Applications

We introduce new methods to generate finite representative collections of plausible yet severe scenarios. We apply these methods to generate credit risk scenarios and demonstrate, via numerical experiments, that with respect to certain performance measures, our method is better able to discover (ex ante) scenarios close to those that occurred (as determined ex post), than previously described methods. Moreover, our methods discover these scenarios at substantially lower computational cost.

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MS24

Stress Testing Model Risk

Abstract not available at time of publication.

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MS24

Must Stress Tests be Credible?

Abstract not available at time of publication.

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MS25

Utility Indifference Pricing in Energy Markets

Abstract not available at time of publication.

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MS25

Probabilistic Approach to Mean Field Games and the Control of McKean Vlasov Dynamics

Abstract not available at time of publication.

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MS25

Levy Semistationary Processes with Applications to Electricity Markets

So called Levy semistationary processes (LSS processes) constitute a rather general class of continuous time moving average processes. Our motivation is employing these processes to model electricity and commodity forwards and spots. We discuss and analyze numerical simulation procedures for LSS processes and energy forward random fields, by means of stochastic partial differential equations, Fourier methods and finite dimensional approximations.

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MS25

Forward-Backward SDE Games and Stochastic Control under Model with Uncertainty

Abstract not available at time of publication.

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MS26

Forward Equations and Mimicking Theorems for Discontinuous Semimartingales

We derive a forward partial integro-differential equation for prices of call options in a model where the dynamics of the underlying asset under the pricing measure is described by a -possibly discontinuous- semimartingale. A uniqueness theorem is given for the solutions of this equation. We relate this result to the construction of a Markovian projection - a Markov process which mimics the marginals distributions of the semimartingale. This result generalizes Dupire's forward equation to a large class of non-Markovian models with jumps.

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MS26

Functional Ito Calculus and the Pricing and Hedging of Path-dependent Derivatives

We provide a brief overview of the Functional Ito Calculus [Dupire 2009; Cont & Fournié 2010], which provides a convenient mathematical framework for analyzing path-dependent functionals of Ito processes, and show that it may be used to derive a 'universal' pricing equation which holds for a wide class of path-dependent options on an underlying asset whose price follows an Ito process. This universal pricing equation is a functional analog of the backward Kolmogorov equation: we present a uniqueness result for solutions of this equation and show that it verifies a comparison principle. Finally, we provide a unified approach to the computation of hedging strategies for path-dependent options.

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MS26

Local Vs Non-Local Forward Equations for Option Pricing

When the underlying asset is a continuous martingale, call option prices solve the Dupire equation, a forward parabolic PDE in the maturity and strike variables. By contrast, when the underlying asset is described by a discontinuous semimartingale, call price solve a partial integro-differential equation (PIDE), containing a non-local integral term. We show that the two classes of equations share no common solution: a given set of option prices is either generated from a continuous martingale ("diffusion") model or from a model with jumps, but not both. In particular, our result shows that Dupires inversion formula for reconstructing local volatility from option prices does not apply to option prices generated from models with jumps.

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MS26

Degenerate Parabolic PDEs, Martingale Problems and a Mimicking Theorem for Itô Processes

We prove existence, uniqueness and regularity of solutions in weighted Hölder spaces for a certain class of degenerate parabolic partial differential equations with unbounded coefficients on the half space. We show that the martingale problem associate with the differential operator is well-posed, which implies existence and uniqueness of weak solutions to the corresponding stochastic differential equations. The weak solutions match the one-dimensional probability distributions of a certain class of Itô processes.

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MS27

Credit Risk Concentration under Stress

We present a general approach to implementing stress scenarios in multi-factor credit portfolio models, which is based on the truncation of risk factors. We derive analytic formulae for credit correlations under stress and analyze their asymptotic behavior in normal variance mixture (NVM) models. It turns out that correlations in heavy-tailed NVM models are less sensitive to stress than in medium- or light-tailed models.

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MS27

Risk Assessment Modelling of Systemic Institutions

The Bank of England has developed a top-down stress testing and systemic risk model (RAMSI). The model contains a network of banks, with each bank modelled in considerable detail. RAMSI allows the banks to be shocked by (deterministic or stochastic) macroeconomic scenarios to determine the resilience of the system under stress. The banks can themselves propagate stress around the system through second round effects. We present the model and an illustration of its use.

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MS27

A Systematic Approach to Multi-period Stress Testing of Portfolio Credit Risk

We propose a new method for analysing multiperiod stress scenarios for portfolio credit risk more systematically than in current macro stress tests. The plausibility of a scenario is quantified by its distance from an average scenario. For a given level of plausibility, we search systematically for the most adverse scenario. We show how this method can be applied to some models already in use by practitioners.

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MS27

Lessons and Limits of Stress Tests as a Macroprudential Supervisory Tool

Abstract not available at time of publication.

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MS28

Derivatives on Non-Storable Renewable Resources: Fish Futures and Options, Not So Fishy after All.

We study forward prices and prices of European call options, which are written on a non-storable renewable resource. An example for such derivatives is provided by futures and options on fresh salmon traded in large volumes at Fish Pool (Norway) since 2008. The introduction of similar exchanges in the United States and other countries is currently discussed. The pricing formulas are derived from first principles, starting of by modeling the dynamics of the resource reserves, and assuming that resource extraction is managed as open access. We derive closed form solutions for the forward price of the renewable resource and study its dynamics. In contrast to Black (1976) we show that forward prices do not evolve according to a geometric Brownian motion, but follow a more complex process. For the case of an option we show that the Black (1976) formula needs to be adapted in such a way, that the normal distribution is replaced by a reciprocal Γ-distribution, to get at least a very good approximation of the true option price. We include numerical evidence to underline this statement. Finally, we derive pricing formulas for options written on forward contracts, and show how forward contracts can be hedged under the assumption that there is a spanning asset. The full paper is available at SSRN: http://ssrn.com/abstract=1469135 The presentation will also include material from a second working paper, which includes more empirical analysis.

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MS28

Adaptations of Least-squares Methods to Convex Control Problems

Abstract not available at time of publication.

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MS28

Dark Pools and Hidden Markets

Abstract not available at time of publication.

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MS28

A Feedback Model for the Financialization of Commodity Prices

Abstract not available at time of publication.

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MS29

A Flexible Matrix Libor Model with Smiles

We present a flexible approach for the valuation of interest rate derivatives based on Affine Processes. We extend the methodology proposed in Keller-Ressel et al. (2009) by changing the choice of the state space. We provide semi-closed-form solutions for the pricing of caps and floors. We then show that it is possible to price swaptions in a multi-factor setting with a good degree of analytical tractability. This is done via the Edgeworth expansion approach developed in Collin-Dufresne and Goldstein (2002). A numerical exercise illustrates the flexibility of the Wishart Libor model in describing the movements of the implied volatility surface.

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MS29

The Explicit Laplace Transform for the Wishart Process

We derive the explicit formula for the joint Laplace transform of the Wishart process and its time integral which extends the original approach of [Bru, M. F. (1991): Wishart processes. Journal of Theoretical Probability, 4:725751]. We compare our methodology with the alternative results given by the variation of constants method, the linearization of the Matrix Riccati ODEs and the Runge-Kutta algorithm. The new formula turns out to be fast, accurate and very useful for applications when dealing with stochastic volatility and stochastic correlation modelling.

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MS29

Generalized Affine Transform Formulae and Exact Simulation of the WMSV Model

The aim of this talk is to introduce transform formulae for linear functionals of affine processes and their bridges whose state space is a set of positive semidefinite matrices. Particularly, we investigate the relationship between such transforms and certain integral equations. We are, then, able to derive analytic expressions for Laplace transforms of some functionals of Wishart bridges. As an application, we suggest an exact simulation method of Wishart multi-dimensional stochastic volatility model.

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MS29

Calibration of Multivariate Affine Stochastic Volatility Models

We provide a new calibration algorithm for multivariate affine stochastic covariance models using both option and timeseries data. The option data is used to recover the parameters determining the drift of the covariance process, while the timeseries allows us to identify the volatility of the covariance process and its correlation to the price processes. The procedure relies only on the knowledge of the first moments of log-prices and an estimation of volatility using Fourier series.

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MS30

Calibrating Volatility Surfaces for Commodity Derivatives

Commodities and their derivatives have become key players in the portfolios of many corporations, especially for those working in the energy sector. In this talk we shall discuss the calibration of local volatility surfaces for commodity derivatives. In order to obtain stable and robust results we shall make use of regularization techniques to handle the inverse problem. In particular we shall present some results with Brent oil (WTI) and Natural Gas (HH) data.

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MS30

Volatility Surface Calibration and Relative-Entropy Minimization

In this talk we will survey the research developed jointly with a number of collaborators during the past few years in connection with the calibration of Black-Scholes models under stochastic volatility. We shall start with the relation between uncertain volatility models, Hamilton-Jacobi equations, and the Kullback-Leibler distance. Then, we shall discuss calibration and entropy. Finally we will discuss weighted Monte Carlo methods and applications.

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MS30

Calibrating Self-exciting Marked Point Processes for Algorithmic Trading

Recently, marked point processes have been used to model the dynamics of assets at ultra-high frequencies. Cartea, Jaimungal and Ricci (2011) develop a multi-factor self-exciting model accounting for the arrival of market orders that influence activity, trigger one- and two-sided clustering of trades, and induce temporary changes in the shape of the LOB. The classification of trades as influential versus non-influential induces hidden state variables and makes online calibration a necessity in high frequency trading a challenging endeavor. Here, we develop quasi-maximum-likelihood parameter estimators and a Sequential Monte Carlo estimator of the activity path for use in algorithmic trading strategies.

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MS30

An Overview of Calibration Methods of Local Volatility Surfaces

Local volatility models are extensively used and well recognized for hedging and pricing in financial markets. They are frequently used, for instance, in the evaluation of exotic options so as to avoid arbitrage opportunities with respect to other instruments. Yet, the ill-posed character of local volatility surface calibration from market prices requires the use of regularization techniques either implicitly or explicitly. Such regularization techniques have been widely studied for a while and are still a topic of intense research. In this talk we shall review different attempts that have been made in order to tackle the local volatility calibration problem. In particular, we shall discuss convex regularization tools and recent inverse problem advances to deal with the calibration problem.

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PP1

Adjoint Monte-Carlo Technique for Calibration of Financial Market Models

We present a Monte-Carlo based adjoint technique for solving calibration problems of financial market models like the Heston model with time-dependent parameters. Any efficient optimization method for calibration requires at least gradient information. The major advantage of the adjoint technique lies in the fact that the calculation time required for a gradient computation stays nearly constant, independent of the number of parameters. Our numerical results confirm this improved speed-up.

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PP1

On Efficient Option Pricing Under Jump Diffusion

Merton's jump-diffusion model leads to partial-integro differential equations (PIDE), which can be solved in order to price options. Discretization of the integral in the PIDE leads to non-local terms and dense matrices. The presentation will discuss ways to solve the PIDE, avoiding dense matrices. This is applied to European-style options.

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PP1

The Impact of Constraints on the Views of the Black-Litterman Model

The Black-Litterman model is a Bayesian portfolio optimization model that allows investors to impose prior views on the expected returns of assets in the portfolio. Constraints can be considered as prior views on the optimal portfolio weights. Constraints distort the views expressed by the investor, resulting in sub-optimal portfolio weights. Our research shows that a mild relaxation of the long-only constraint results in Black-Litterman views that are more efficiently represented in the portfolio weights.

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