IC1

Optimization Modeling: Recent Enhancements and Future Extensions

Modeling systems are an efficient way to develop the constraints and objectives for optimization and equilibrium problems. We outline several recent enhancements of such systems that facilitate grid solution techniques, complementarity or equilibrium constraints within optimization problems, model embedding, and explicit formulation of stochastic constraints and extended nonlinear programming problems. Further extensions of these systems to ease the modeling burden in specific contexts will also be proposed, along with computational results in particular application domains.

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IC2

Multiscale Methods for Dilute Fluids and Plasmas

Monte Carlo particle methods have been used with great success for fluid and plasma flows in which collisional effects are significant. Applications range from flight in the upper atmosphere to the lubrication of a hard disk and the edge region in a fusion plasma. In the near fluid regime, however, the particle collision rate becomes very large, so that particle methods can become computationally intractable. Hybrid methods combining discrete and continuum (i.e., particle and fluid) descriptions are a promising alternative that can retain the accuracy of a full particle method and the speed of a fluid dynamic solver. The formulation and analysis of these methods depends significantly on the fluid dynamic limit for kinetic theory. This talk describes the mathematical basis and computational performance for several different hybrid methods.

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IC3

Mathematical Neuroscience: From Neurons to Networks

The tools of dynamical systems theory are having an increasing impact on our understanding of patterns of neural activity. In this talk I will describe how to build tractable tissue level models that maintain a strong link with biophysical reality. These models typically take the form of nonlinear integro-differential equations. Their non-local nature has led to the development of a set of analytical and numerical tools for the study of waves, bumps and patterns, based around natural extensions of those used for local differential equation models. Here I will present an overview of these techniques.

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IC4

The Parallel Revolution in Computational Science and Engineering

The computer industry is going through an exciting, disruptive transformation by switching to massive parallelism in processor design. Today, more than 100 million computers are running parallelized applications 20-100 times faster than their sequential versions. By year 2016, parallelism could provide over 1,000 times speedup. Such a dramatic increase in computation power has already enabled revolutionary work, or time warp, in science and engineering disciplines. This talk aims to offer insight into the opportunities that these inexpensive parallel computers offer to researchers and how some disciplines are already benefiting from the revolution.

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IC5

The Design and Analysis of Multithreaded Algorithms

This talk overviews multithreaded algorithmic design as supported by the Cilk++ concurrency platform. Cilk++ allows a programmer to analyze algorithms in terms of the theoretically elegant notions of work and span, whose ratio provides a quantitative measure of parallelism. The performance of a Cilk++ program is mathematically guaranteed to scale up linearly with the number of processors, as long as the application exhibits sufficient parallelism and the computer architecture provides sufficient memory bandwidth. Example problems that admit efficient parallel algorithms in both theory and practice include Strassen's matrix-multiplication algorithm, sparse matrix-vector multiplication, sorting, and breadth-first search of a graph.

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IC6

Optimization: The Difference Between Theory and Practice

Theres an old saying, In theory, theres no difference between theory and practice, but in practice there is. Today, scientists are working on optimization problems arising in fields such as nanoscience, astrophysics, and the electric power grid. The resulting simulation-based optimization problems have different characteristics than classical problems and usually require different theoretical assumptions. In this talk, I will discuss challenges one faces when solving these optimization problems and what roles theory and practice play in developing new algorithms. I will present several techniques for simulation-based optimization problems and some lessons learned in applying theory to practical problems.

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IC7

Combinatorics Inspired by Biology

Mathematics has played an important role in biology, both as a useful language for modeling biological phenomena, and in the tools it provides for data analysis. The flood of data that is now emerging from the transformation of biology into a high-throughput science makes mathematics particularly relevant for biologists at this time. In this talk we will not emphasize the role of mathematics in biology, but rather we focus on the impact biology has had on mathematics. Using a few key examples that are well known to biologists (but maybe not as much to mathematicians), we will highlight a few key ideas in combinatorics that were inspired by biologists.

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IC8
Modeling Cancer-Immunology Dynamics

Immunotherapy, a treatment approach that enhances the body's natural ability to fight cancers, is becoming increasingly prevalent in many multi-stage treatment programs that also include chemotherapy, radiation and surgery. The critical importance of the immune system in combating cancer has been verified both clinically and through mathematical models. In this talk, we will discuss the biological and mathematical sides of the question of how cancer grows, how the cancer interacts with the immune system, and treatment approaches that harness the power of the immune system.

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IC9
Controlling Lagrangian Systems by Active Constraints

The talk will survey past and recent work on the stabilization and control of mechanical systems, by imposing a number of time-dependent, frictionless constraints. The basic mathematical description involves a Riemann manifold, together with a foliation describing the constraints. The equations of motion usually have an impulsive character, containing the time derivatives of the control functions. Their analytical form is closely linked to the geometrical structure of the foliation. We observe that this same framework can also be used to study swim-like motion of one or more deformable bodies in a perfect fluid.

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IC10
Parallel Implicit Nonlinear Solvers in Large-Scale Computational Science

Parallel implicit solution strategies have proven robust and efficient in resolving challenging nonlinearities in many large-scale PDE-based simulations. We discuss the use of preconditioned Newton-Krylov methods for parallel applications in coupled core-edge plasma and multiphase reactive flow, with emphasis on capabilities in the PETSc library that enable users to leverage domain-specific legacy code and to exploit library-provided functionality for sparse derivative computations and scalable preconditioners. We highlight complementary capabilities of additional software in the Towards Optimal Petascale Simulations (TOPS) project, with emphasis on how such software provides robust, scalable, and extensible capabilities that are increasingly important for multimodel and multiphysics simulations on emerging high-performance architectures.

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IC11
Some Stochastic Control Problems in Mathematical Finance

We formulate a class of stochastic control problems, collectively known under the rubric of portfolio optimization, that arise in the mathematics of finance. Ideas from convex duality play a prominent role in their resolution; so do parabolic partial differential equations, under strong conditions on the financial market structure. Under less stringent conditions, stochastic analogues of the classical Hamilton-Jacobi-Bellman equation emerge as particularly relevant in this context, in connection with results from backwards stochastic equations and the Ito-Wentzell formula for random fields. Using such tools, feedback formulae become available for the investors optimal strategies, based on his current level of wealth. Recent progress on these issues will be surveyed, and some open questions will be mentioned.

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IC12
Parallel Network Analysis

We consider methods for the parallel solution of graph-based and combinatorial problems arising in the design of sensor networks or the analysis of social networks. While some aspects of these applications have obvious partitions with "embarrassing" parallelism, the lack of locality when searching through graph neighborhoods has historically made parallelization of graph algorithms difficult. A new generation of massively multithreaded parallel computers is well suited for algorithms with significant memory latency, provided there is sufficient total parallelism. We will discuss algorithmic techniques for solving graph problems on such architectures including a powerful primitive originally developed for the Connection Machine CM-2 and Lagrangian techniques originally developed for low-memory PCs.

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IC13
Progress Toward a Stability Proof for Scott Russell's Solitary Wave

A classic story of nonlinear science started with the particle-like water wave that Russell famously chased on horseback in 1834. Nowadays the theory of solitons in integrable PDE is highly developed and nonlinear pulses compete for a prominent role in optical communications technology. Yet the dynamics of many nonlinear waves remain rather ill-understood. I will recount progress regarding the robustness of solitary waves in nonintegrable model systems such as FPU lattices, and discuss a draft proof (with Shu-Ming Sun) of spectral stability of small solitary waves for the 2D Euler equations for water of finite depth without surface tension.

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IC14

On the Complexity of Game, Market, and Network Equilibria

As you may have already known, the notion of the Nash equilibrium has captured the imagination of much of the computer science theory community, both for its many applications in the growing domain of online interactions and for its deep and fundamental mathematical structures. As the scale of typical internet applications increases, the problems of efficiently analyzing their game-theoretic properties become more pointed. I will discuss some of our recent results in settling several open questions about Nash equilibria of matrix games and Arrow-Debreu equilibria of exchange markets. I will also address the extensions of these results to other equilibrium problems that arise in collaborative games and in the game-theoretic studies of the Internet BGP protocols. Joint work with Xi Chen (Princeton), Xiaotie Deng (The City University of Hong Kong); also with Li-Sha Huang (Google China), Paul Valiant (MIT), Kyle Burke (Boston University), Shiva Kintali (Georgia Tech), Laura J. Poplawski (Northeastern), Rajmohan Rajaraman (Northeastern), and Ravi Sundaram (Northeastern).

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IP0

AWM-SIAM Sonia Kovalevsky Lecture: Swarming by Nature and by Design

The cohesive movement of a biological population is a commonly observed natural phenomenon. With the advent of platforms of unmanned vehicles, such phenomena has attracted a renewed interest from the engineering community. This talk will cover a survey of the speaker's research and related work in this area ranging from aggregation models in nonlinear PDE to control algorithms and robotic testbed experiments. We conclude with a discussion of some interesting problems for the applied mathematics community.

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IP0

The John Von Neumann Lecture

To follow.

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IP0

W. T. and Idalia Reid Prize in Mathematics Lecture: The Moment Problem for Positive Rational Measures: Convexity in the Spirit of Krein

The moment problem as formulated by Krein and Nudel'man is a beautiful generalization of several important classical moment problems. However, the importance of rational functions in systems and control and other engineering applications imposes certain complexity constraints. In this talk we present a new formulation of the moment problem which respects these constraints. While this version of the problem is decidedly nonlinear, the basic tools still rely on convexity. In particular, we present a solution in terms of a convex optimization problem that generalizes the maximum entropy approach used in several classical special cases.

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IP0

I.E. Block Community Lecture: "Kill All The Quants?": Models vs. Mania In The Current Financial Crisis

As the shockwaves of the financial crisis of 2008 propagate throughout the global economy, the "blame game" has begun in earnest, with some fingers pointing to the complexity of certain financial securities, and the mathematical models used to manage them. In this talk, I will review the evidence for and against this view, and argue that a broader perspective will show a much different picture. Blaming quantitative analysis for the financial crisis is akin to blaming $E = MC^2$ for nuclear meltdowns. A more productive line of inquiry might be to look deeper into the underlying causes of financial crisis, which ultimately leads to the conclusion that bubbles, crashes, and market dislocation are unavoidable consequences of hardwired human behavior coupled with free enterprise and modern capitalism. However, even though crises cannot be legislated away, there are many ways to reduce their disruptive effects, and I will conclude with a set of proposals for regulatory reform.

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IP0

Past Presidents Address: Parallelism and Puzzles

Every talk that Ive given at a SIAM meeting for the past 30 years has included some material about parallel computing. This talk will be no exception. In addition, I want to demonstrate some of our Experiments with MATLAB project intended for younger students.

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IP0

Theodore Von Karman Prize Lecture: Computational Environments for Coupling Multiphase Flow, Transport, and Geomechanics in Porous Me-

dia for Modeling Carbon Sequestration

Geologic sequestration by injection of CO2 into deep brine aquifers and reservoirs represents one of the most promising approaches for reducing atmospheric CO2. 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. We present a "wish list" for simulator capabilities and describe algorithms and software being developed at UT-Austin.

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IP1

Computational Geosciences: A Perspective from Geological Basin Modeling

The modeling of geological processes operating in a time-scale of millions of years during the formation and evolution of sedimentary basins is formidable challenge due to its mutiphysics, multiscale, and computational characteristics. In this presentation I will discuss the issues related to mathematical modeling, simulation, data analysis, uncertainty, and high performance parallel computing, from the basin modeling perspective with an historical angle. Basin modeling is an essential tool for the understating the formation of major mineral and hydrocarbon resources.

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IP2

Initial Boundary Value Problems for Second Order Systems of Partial Differential Equations

Problems concerned with wave propagation in two or three space dimensions are often formulated in terms of systems of wave equations which we have to solve numerically. Examples are Maxwell's equations, elastic wave equations and Einstein's equation of general relativity. We want to solve the initial boundary value problems for $t \geq 0$ in a finite domain Ω in space with a smooth boundary Γ. At $t = 0$ we give initial conditions and on Γ boundary conditions which are either Diriclet conditions or relations between normal and tangential derivatives. The most desirable properties for these problems is that there is an energy estimate and that the problem is stable against lower order perturbations. The usual way to prove the existence of an energy estimate is by integration by parts. This is always possible for the Cauchy problem and problems with Diriclet boundary conditions. In these cases the numerical solution poses relatively few difficulties. Physical phenomena like glancing or surface waves lead to derivative boundary conditions which are not maximally dissipative. The energy estimate does not give us a detailed understanding about the behavior of the solution near the boundary which is desireable to develop numerical techniques. By solving a Cauchy problem we can reduce the data such that only the boundary conditions are inhomogeneous. Also, the required stability estimates are such that we can reduce the discussion to halfspace problems. For halfspace problems we will discuss a theory which is based on Fourier and Laplace transform which gives us the desired information about the solution and apply it to the earlier mentioned equations.

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JP1

Semi-smooth Newton Methods in Function Spaces and Applications to Variational Problems in Optimal Control and Imaging

Non-differentiable variational problems arise in diverse areas of current interest, as for instance in optimal control governed by partial differential equations with constraints on the controls or the state, in mathematical imaging with bounded variation (BV) type regularization or sparsity constraints, in mathematical finance, and control of variational inequalities. At first, second order Newton type methods appear to be out of scope, and therefore (conjugate-) gradient methods are often used to solve such problems in practice. Exploiting the special structure, however, frequently *Newton-differentiability* can still be ascertained. This guarantees super-linear convergence of Newton-type methods. In case Newton-differentiability fails this is a phenomenon of the infinite dimensional setting and can be remedied by a regularization process. For the choice of the regularization parameter a model-based path-following strategy is proposed.

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CP1

Possibly New Methods for Evaluating Bessel Integrals and Series

Known results of integrals and series involving Bessel functions currently avaliable in handbooks, but we found no recourse in the well- known refferences to how they were established. In the first part of this paper we introduce a possibly new method for evaluating Bessel integrals by identifying a certaint type of differential equations. In the second part of this paper we suggest a possibly new Method for evaluating a class of schlomilch type series. The paper concludes by indicating the wide range of results that can be established.

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CP1

Physical Modeling, Field Oriented Control Analysis of An Ac Machine

This work deals with the study of Maxwell's equations arising by creation of electromagnetic fields in an electric machine which could be a transformer or an Induction machine. The structure of these two machines could be similar though behavior in some sense may not be same. For example Induction machine can be used for a design which solely requires for heating purpose. The transformer may be used to transfer large amount of power, voltage. In present case we consider the machine windings for homogeneous or nonhomogeneous medium with Dirichlet and Mixed Boundary conditions. We study time independent equations first and compare it with time dependent equations. Many cases of time dependent as well as time independent Rotor and Stator equations for three phase machines have been studied before. A comparison of exact solutions to numerical solutions is established for different layers of transformer windings under different structure. We further look for extra stator losses and eddy currents produced and the loss of power. A Power-current or skin depth plot and that Torque-skin depth plot will be done to find out how to control and minimize the power loss and increase amount of torque required to start the machine or stop the machine in no time by using transient analysis and classical NYQuist and Bode plots. In other words we find torque to be controlled b filed oriented control. An example is under consideration that will depict how equations and solutions behave differently in different media/materials with respect to power and torque control. The analysis is being done by using combination of software. These are Femlab, Mat-lab and Simulink and SCILAB.

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CP1
Numerical Conformal Mappings onto the Linear Slit Domain

We propose a numerical method for the conformal mapping of unbounded multiply-connected domains exterior to closed Jordan curves onto a canonical linear slit domain, which is a generalization of the well-known parallel slit domain. The method is based on the charge simulation method (the fundamental solution method), and gives a simple form of approximate mapping functions with high accuracy.

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CP1
Polygons and Circles in Computational Science

The area between a unit circle and an inscribed n-sided regular polygon is not hard to compute. What is important is that this "change in area" gives the leading term in the difference in the eigenvalues of the Laplacian for polygons and circles. This leads to a practical suggestion for the eigenvalue problem (and for other problems too): Let the polygon go outside the circle enough to have the same area. Then the error from changing to a polygon and creating a mesh and solving by finite elements is much reduced. (The next term in the eigenvalue error was found by Pavel Grinfeld and it involves the Riemann zeta function...)

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CP1
Four Bugs on a Rectangle

Four bugs start at t=0 at the vertices of a 2x1 rectangle. Each one chases the bug to its left with speed 1. What's the shape of the ensuing spiral? You may think this sounds like a problem made famous by Martin Gardner in Scientific American, but it is remarkably different because of the rectangular initial condition. This talk will describe the bugs' extraordinary paths with the help of some unusual asymptotic analysis, joint work with James Lottes and S. J. Chapman. By the time the first circuit of the origin is completed, the scale of the configuration has shrunk by a factor of exp(exp(25))!

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CP2
Modeling Framework for Fluid-Solid Mixtures Using Distinct Phases and the Material Point Method

Partially and fully saturated porous media have been a research focus for several decades. The most common simulation approaches are based on homogenization techniques to obtain continuum-like formulations enriched by, e.g., pressure variables for embedded fluid phases. While proven very successful for solid dominated problems, such models present tough challenges as the mixture undergoes a transition from solid-like to fluid-like behavior. The present paper proposes to model solid and fluid phases as distinct matter using specialized particles for each phase within the framework of the material point method (MPM). Mixture behavior is obtained by introducing drag terms for momentum transfer and a volume constraint to assess the effect of confining pressure in fully saturated media. The paper presents the basic ingredients which, in combination with the established MPM, will yield a generic framework for a wide variety of problems incorporating fluid-solid mixtures.

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CP2

Theory of Particle Heat Transfer in Gas-Solid Systems Applied to Discrete Element Methods (dem)

There are various theories for calculating the heat transfer in particles of gas-solid systems. A brief review of these concepts along with the advantages and disadvantages surrounding their incorporation into a discrete element method (DEM) model are presented.

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CP2

Fluid Structure Control Interactions For Coupled Problems

The problem of efficient modeling and simulation of the interaction of fluid with a solid undergoing nonlinear deformation has remained a challenging problem in computational science and engineering. The purpose of this talk is to introduce a computational methodology using finite elements that offers the flexibility and efficiency to study coupled problems involving fluid-structure interaction. An Arbitrary Lagrangian-Eulerian (ALE) formulation is used to move the mesh at each time step. This approach avoids excessive deformation of the mesh near the fluid-structure interface that may occur due to transient dynamic loads. Numerical computations will be presented to validate the performance of the method for benchmark applications involving fluid-structure interaction. Theoretical and computational performance of such problems formulated as optimal control problems will also be presented.

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CP2

Efficient Numerical Computation of Fluid Interfaces with Soluble Surfactant

We address a significant difficulty in the numerical computation of fluid interfaces with soluble surfactant that occurs in the practically important limit of very large values of bulk Peclet number Pe. At the high values of Pe in typical fluid-surfactant systems, there is a transition layer near the interface in which the surfactant concentration varies rapidly, and its gradient at the interface must be determined accurately to find the drop's dynamics. Accurately resolving the layer is a challenge for traditional numerical methods. We present recent work that uses the slenderness of the layer to develop a fast and accurate 'hybrid' numerical method that incorporates a separate analytical reduction of the dynamics in the transition layer into a full numerical solution of the interfacial free boundary problem.

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CP2

Free Boundary Problem for a Supercavitating Wedge

Motion of a yawed supercavitating wedge under a free surface and in a jet of an ideal liquid is analyzed. The Tulin-Terent'ev cavity closure mechanism and the theory of Riemann surfaces are used for the description of the flow around the cavity. A conformal map from a plane with two cuts into the doubly connected flow domain is constructed by solving two Riemann-Hilbert problems on a genus-1 Riemann surface.

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CP3

Nonlinear Breathing Modes at a DNA Defect Site

We develop a stochastic mesoscopic model of a DNA duplex, with parameters fitted to AMBER data for different twist angles (in the range 30°-40°). With a 'rogue' difluorotoluene base at the defect site, breathing events - the temporary breaking of bonds between complementary bases - occur more frequently, that is, on the nanosecond timescale. We discuss fluctuation-dissipation relations, energy barriers, the potential of mean force and potential energies in reduced models.

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CP3

A Dynamical Model of Exit From Mitosis in Budding Yeast

Exit from mitosis requires activation of Cdc14, an essential phosphatase promoting mitotic exit. We have developed a deterministic ODE model for the control of Cdc14 release as the cells exit from mitosis. Our model provides a rigorous account of the factors affecting the dual exit pathways, called FEAR and MEN. The model captures the dynamics of mitotic exit in wild-type and mutant cells, including many details of the physiology, biochemistry and genetics of the process.

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CP3

Emergent Dynamics Governed by Regulatory Cells Produce a Robust Primary T Cell Response

Several theories exist concerning primary killer T cell responses, the most prevalent being that T cells follow developmental programs. We propose the alternative hypothesis that the response is governed by a feedback loop between conventional and regulatory T cells. By developing a mathematical model, we show that the regulated response is robust to a wide variety of parameters and propose that T cell responses may be governed by emergent group dynamics rather than by autonomous programs.

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CP3

Dynamic Bayesian Network Modeling of Gene Expression Data

We report our recently developments in network modeling of gene expression data using the dynamic Bayesian network approach. This includes incorporating existing biological information (co-citation, GO similarity, positional and binding information, etc) as prior knowledge, fuzzy theory-based rules to the MCMC learning of DBYN, definition of gene expression (phase) synchronization module and utilization of it it to assist initial network structure construction, etc. We show that these lead to significantly improved performance, through application to the microarray study of pancreatic development.

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CP3

Mathematical Study of Islet Bursting and the Dependence on the Cytoarchetectural Organization of Iset Cells

We report our mathematical development to study the spatial-temporal regulation of insulin release from pancreatic islet beta cells. An islet can be mathematically modeled as a networks of nonlinear oscillators (beta cells) coupled through gap junctions and various chemicals, and the robust oscillatory insulin release is an emergent phenomenon. Using both ODE and PDE systems, we study the synchronization, pattern formation, wave front propagation and noise-induced orders in the islet of coupled non-linear stochastic systems, and from the results derive mathematical models of beta-cell function

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CP3

The Stochastic Simulation of the FtsZ Ring Assembly and Contraction

In a previous research, a biochemical reaction network is developed to simulate the assembly and contraction of the FtsZ ring. We investigate its stochastic behavior since numbers of long open polymers and closed rings are mostly small (¡10). A modified next reaction method is used. The results are compared with those obtained with deterministic model. For the assembly process, the two simulations only show small difference. However, qualitative differences appear for the contraction process.

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CP4

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

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

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CP4

The Estimation of the Effective Reproductive Number from Disease Outbreak Data

We consider a single outbreak susceptible-infected-recovered (SIR) model and corresponding estimation procedures for the effective reproductive number $\mathcal{R}(\sqcup)$. We discuss the estimation of the underlying SIR parameters with a generalized least squares (GLS) estimation technique. We use asymptotic statistical theories to derive the mean and variance of the limiting sampling distribution and to perform post statistical analysis of the inverse problems. We illustrate the ideas and pitfalls with both synthetic and influenza incidence data sets.

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CP4

Spatial Propagation of Alleles in a Human Population

We seek to model the spatial propagation of alleles through a population using modified Fisher-Kolmogorov Equations in one and two dimensions. We will present preliminary results of our investigation into the analysis and simulation of solutions to our model. We will also discuss our investigation into the inverse problem of identifying the propagation speed as well as geographic barriers to migration. We apply our mathematical model to study allele distributions in human populations.

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CP4

A Coalescent Analysis of Genetic Statistics Used in Population Subdivision Inference

Populations are often divided into subpopulations. Biologists use various statistics formed from genetic data to infer migration rates between subpopulations. In this talk we consider such statistics under a certain class of evolutionary models. We use coalescent theory to derive the distribution of a certain subset of such statistics. We then use our results to comment on an important question: Can the shape of a subdivided population be determined from genetic data?

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CP4

Competition and Disease Dynamics in Multi-Species Interactions

It has been shown that disease can modulate competition between multiple host species and can be a major factor in invasion by exotic species. We model and analyze the dynamics of multi-host communities using Lotka-Volterra full competition, which affects birth rates of species, and Susceptible-Infected disease dynamics, to understand how the forces of inter-specific infection and competition combine to allow invasion by exotic species. For the case of two species we analyze the disease free equilibrium for stability and for the case of disease transmission via frequency incidence we consider the stability of the endemic coexistence equilibrium. We also extend some threshold values to the case of multiple species.

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CP5

A Uniqueness Question Relating to Thermo-Acoustic Tomography and Reconstruction in the Radially Symmetric Case

A new result pertaining to a mostly unexplored uniqueness question in thermo-acoustic tomography is presented. We demonstrate a partial answer to the question, If $u_1(x,t)$ and $u_2(x,t)$ satisfy

$$\begin{aligned}
\partial_t^2 u_1 - c_1^2(x)\Delta u_1 &= 0 \text{ in } \mathbf{R}^n \times \mathbf{R}_+ \\
\partial_t^2 u_2 - c_2^2(x)\Delta u_2 &= 0 \text{ in } \mathbf{R}^n \times \mathbf{R}_+ \\
u_1(x,0), u_2(x,0) &\in C_0^\infty(D), \\
\partial_t u_1(x,0) = 0 &= \partial_t u_2(x,0) \text{ in } \mathbf{R}^n \\
u_1(x,t) &= u_2(x,t) \text{ on } \partial D \times \mathbf{R}_+
\end{aligned}$$

then is $c_1(x) = c_2(x)$ in D? We use the relation of the wave equation to the Helmholtz equation and decay estimates for the wave equation to show that uniqueness of the sound speed is connected to the interior transmission problem. Techniques for the reconstruction of the sound speed and initial impulse in thermo-acoustic tomography are shown for a radial symmetric problem.

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CP5

Conditional Well-Posedness for An Elliptic Inverse Problem

The inverse elliptic equation $-\nabla \cdot (p(x)\nabla v) + \lambda q(x)v = f,\ x \in \Omega \subset \mathbf{R^n}$, is important in groundwater modeling. The problem of determining when one or more of the coefficient functions p, q, and f depends continuously on the solution functions $v = v_{p,q,f,\lambda}$ is considered. We establish conditions required for weak-$L^2(\Omega)$ continuity of q and f and ∇v-weak $L^2(\Omega)$ continuity of p, given $H^1(\Omega)$ continuity of v.

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CP5

Multilevel Domain Decomposition Algorithms for Inverse Elliptic Problems

We investigate scalable multilevel domain decomposition algorithms for solving inverse elliptic problems formulated as optimization problems constrained by partial differential equations. To solve these optimization problems, we employ a fully coupled Lagrange-Newton-Krylov-Schwarz algorithm. One of the key steps in the algorithm is the Jacobian preconditioning, for which we study and compare four types of two-level domain decomposition methods. Our numerical results show that the algorithms work well for different types of observations in terms of the accuracy of the solution, and some of the algorithms scale better than the others when the number of processors is large. We also study and report the sensitivity of the algorithms with respect to the jumps of the coefficients, the level of noise in the observed data, the size of the computational domain, the size of the mesh, and the number of processors.

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CP5

Recovering Doping Profiles in Semiconductor Devices with the Boltzmann-Poisson Model

In inverse problem of semiconductor devices, one intends to identify device doping profile from measurement of the device characteristics. The problem has been extensively studied in the past decade. We present in this talk some analytical and numerical studies of the doping profile recovering problem based on the Boltzmann-Poisson model for electron transport in semiconductors. We will make detailed numerical comparison between reconstructions based the Boltzmann-Poisson model and those based on the drift-diffusion model.

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CP5

Numerical Recovery of a Boundary Condition in An Inverse Sturm-Liouville Problem

It is well known that spectral data consisting of an eigenvalue sequence and associated norming constants uniquely determines a potential in a Sturm-Liouville problem, together with one of the boundary conditions in the direct problem. However numerical approaches to the inverse Sturm-Liouville problem which have been developed tend to regard all boundary conditions as known. In this talk I will discuss modification of a particular numerical approach to allow for an unknown boundary condition. An application to the inverse Sturm-Liouville problem for a singular potential will be given.

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CP6

Capillary Gravity Surface Waves by a Positive Forcing

We consider forced surface waves on an incompressible, inviscid fluid in a two-dimensional channel with a small obstruction on a horizontal rigid flat bottom are studied when surface tension is considered. The wave motion on the free surface is determined by a nondimensional wave speed F, called Froude number, and F=1 is a critical value of F. If F=1 + lambda with lambda ¿0 a small parameter, then a time-dependent forced Korteweg de Vries (FKdV) equation can be derived to model the wave motion on the free surface. Here, the case F ¿ 1, called supercritical case, is considered. The solutions of KdV equation with positive forcing are studied theoritically and numerically with zero or nonzero initial conditions .

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CP6

An All-Speed Asymptotic-Preserving Method for the Isentropic Euler Equations

In low-Mach number flows, compressible solvers require high resolution in space and time due to the presence of fast acoustic waves. We propose a semi-implicit splitting of the isentropic Euler equations that formulates the fast terms as an implicit linear system, which can be computed with a Poisson solver, and computes the slow terms explicitly. This method is stable for any Mach number, and captures the correct incompressible limit at the discrete level.

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CP6

Large-Eddy Simulation of Turbulent Combustion

In recent years, large-eddy simulation (LES) has been increasingly and successfully applied to both premixed and non-premixed reacting flows . The present research concerns the numerical prediction of turbulent swirling reacting flows, using the large-eddy simulation (LES) approach. The study shows that LES together with a laminar flamelet model provides a good prediction of the structure of turbulent swirling flames, involving vortex breakdown, flow instability, and the occurrence of localized extinction.

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CP6

A High Order Compact Navier-Stokes Solver on Non-Rectangular Domains

In the present paper, we develop a fourth order compact finite difference method for solving the biharmonic formulation of the Navier-Stokes (N-S) equations. This formulation, which makes use of conformal mappings can be used on geometries beyond rectangular. It is tested on three different problems, namely, (i) fluid flow in a constricted channel, (ii) driven polar cavity and (iii) flow past an impulsively started circular cylinder. The scheme is seen to capture very efficiently the steady-state solutions of the N-S equations with Dirichlet as well as Neumann boundary conditions. We present our numerical results and validate them by comparing with established numerical and experimental results available in literature. Excellent comparison is obtained in all the cases.

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CP6

Mass Flow and Thermal Transfer in a Wide Channel: a Variational Approach to Solve a a Free Boundary Problem

At a certain location of a channel, water is pumped out continuously (sink, as coolant. The heated water is dumped back to the chanel at a further location along the flow direction (source). The minimum distance between source and sink that insures water temprature steadiness, in the sense that temprature at the sink does not rise, is found by solving a free boundary problem, using variational techniques. Validity of the results is checked by finite differences methods.

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CP7

A Proper Orthogonal Decomposition-Based Augmented Conjugate Gradient Algorithm for Nearby Problems

A novel augmented conjugate gradient algorithm is presented for the fast solution of consecutive linear systems of equation of the form $A^i x^i = b^i$, where A^i are nearby symmetric positive definite matrices. Such systems arise in many engineering applications, particularly in optimization. The algorithm augments the Krylov subspace with a proper orthogonal decomposition subspace that approximately minimizes the orthogonal projection error of the solution, thereby accelerating convergence.

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CP7

Effects of Boundary Conditions on Preconditioning Strategies for the Navier-Stokes Equations

Block preconditioners for the linearized Navier-Stokes equations have shown great potential as the basis of efficient iterative solution algorithms. In the derivation of these techniques, boundary conditions have not played a prominent role. We show that boundary conditions can be used to construct improved preconditioners by improving the quality of certain commutators used in the derivation. A new, Robin, condition for preconditioners for problems with velocities satisfying inflow boundary conditions leads to dramatically improved performance.

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CP7

Parallel Algorithms for Sparse Matrix Inverse and Sparse Linear Systems

Computing sparse matrix inverse is critical in many applications including quantum transport in nano-devices. We propose two parallel algorithms for such applications based on ideas from cyclic reduction, dynamic programming, and nested dissection. They are the first parallel algorithms with significant speedup for 2D devices and also faster than other parallel algorithms for 1D devices. A similar parallel algorithm for sparse linear systems with repeated right hand sides with significant speedup was also developed.

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CP7

A Novel Sparse Linear System Solver

We propose a hybrid sparse system solver for handling linear systems using domain decomposition-based techniques. The scheme implicitly imposes an overlapped block diagonal structure on the matrix. Using a modified iterative method a balance system is solved and an adjustment of the right-hand-side is found such that the solution of adjacent blocks matches in the overlapping regions. Finally, the resulting smaller linear systems are solved independently in parallel. This scheme takes advantage of mixed distributed and shared memory platforms and can be used as a standalone solver or as a preconditioner for an outer iterative method. Numerical experiments will be presented.

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CP8

Three Dimensional Discharging Structure of a Mountain Thunderstorm

Recently, wide band measurements of the electric field in a thunderstorm have been obtained by a balloon-borne electric field sonde or Esonde. The data from the Esonde can be combined with simultaneous LMA measurements of VHF pulses emitted during lightning breakdown processes to estimate the charge transport associated with lightning. In this paper, we further enhance the techniques we have developed to process Esonde data by taking better account of instrument rotation,and by computing the local horizontal electric field, not just the lightning induced electric field change. Using these techniques, we analyze lightning charge transport for a thunderstorm which occurred on August 18, 2004, near Langmuir Laboratory, New Mexico. The analysis yields the three dimensional discharging structure of the thunderstorm.

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CP8

Efficient Multigrid Preconditioning for Systems Arising in Solving Large-Scale Inverse Problems with Bound-Constraints Using Interior Point Methods

In this work we address the question of efficiently solving the minimization problem $\min \frac{1}{2}\|Ku-f\|^2+\frac{\beta}{2}\|u\|^2$, subject to the constraints $u \geq 0$, where K is a compact operator. We show that the linear systems arising in the application of interior point methods to the above problem can be solved efficiently using multigrid techniques similar to the ones used for the associated unconstrained problem, which represents the Tikhnov regularization of the ill-posed problem $Ku = f$.

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CP8

Solving Quadratic Knapsack Problem with An Efficient Pegging Algorithm Using Bounds of Dual Variables

We propose an efficient pegging algorithm for solving continuous quadratic knapsack problem (QKP) with box constraints. The problem we address is to minimize a convex and differentiable quadratic function with just one equality constraint and bounds on the variables. Two main approaches for solving this problem are Lagrange multiplier search method as a dual algorithm and variable pegging method as a primal algorithm. Pegging algorithm needs to calculate primal variables to check bounds on variables at each iteration, which frequently is time-consuming. Our newly proposed dual bound algorithm checks the bounds of Lagrange multiplier corresponding to primal variables without calculating primal variables at each iteration. Our experimental results have shown the proposed algorithm has better solution time than the Bitran-Hax algorithm.

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CP8

A Homogeneous Model for Mixed Linear Complementarity Problems

We introduce a homogeneous model for mixed linear complementarity problems which represent a generalization of the standard linear complementarity problems. Without having any regularity assumption concerning the existence of optimal, feasible or interior feasible solutions of the original problem, the homogeneous model is able to provide the solution if it exists, or a certificate of infeasibility, otherwise. We also show that the homogeneous problem can be efficiently solved using interior-point path-following methods and present numerical experiments.

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CP8

Study of Particle Swarm Optimization Formulations for the Solution of Constrained Nonlinear Optimization Problems

This paper presents a study of two current particle swarm formulation approaches which had been formulated to directly handle constraints, the Non-Linear Constrained Particle Swarm Optimization Algorithm and the Augmented Lagrangian Particle Swarm Optimization Algorithm. The functionality and characteristics of each approach are shown and their effectiveness in solving constraint optimization problems is illustrated on different optimization tasks.

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CP9

Optimization Methods for Compressed Sensing in Photon-Limited Imaging

Low-light imaging, which arise in many applications such as infrared and night vision, has the potential to be dramatically impacted by compressed sensing (CS). However, current models used in CS literature do not accurately model the effects of Poisson noise, a common model for photon-limited data. In this talk, we present an optimization approach for minimizing an objective function that allow for the positive and signal-dependent nature of Poisson noise.

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CP9

Continuity and Approximation Order of Boundary Wavelets

Boundary functions for wavelets on a finite interval are usually constructed as linear combinations of standard (interior) scaling functions. Such boundary functions obviously inherit the smoothness properties of the interior functions. Boundary functions can also be constructed directly from recursion relations. We explain how to determine continuity and approximation order in this case. An example shows that this second approach is more general than the first.

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CP9

A New Stochastic Variational Pde Model for Soft Mumford-Shah Segmentation and Denoising

In this talk, we present a new model for soft Mumford-Shah segmentation and denoising for mixture image patterns. We construct a functional with variable exponent which combines the TV-based and isotropic diffusion and we allow each pixel to belong to each image pattern with different probability. By taking different Gaussian means and variances on each image pattern, the segmentation can be more efficient and accurate. Numerical examples of synthetic and natural images are presented to ilustrate the use of the model.

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CP9

Rank-One Perturbation of a Rotation Matrix

In imaging, a homography matrix relates the images of a single scene captured by two different cameras. A homography is a rank-one perturbation of a rotation matrix. The constituent rotation and rank-one perturbation reveal the relative rotation and translation of the two cameras. A classic 1982 paper of Tsai, Huang, and Zhu gave a geometric analysis and provided a computational prescription for computing these constituents given the homography. This work provides an alternative, linear algebraic analysis, revealing other aspects of the problem, and leads to a computational procedure that is robust in corner cases, unlike the formulas of Tsai.

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CP9

Symmetric Eigenfaces

The singular value decomposition (SVD) is the foundation of many algorithms in facial analysis. We generalize the SVD to take advantage of the mirror symmetry that is inherent in faces to create a new facial recognition algorithm, the symmetry preserving singular value decomposition (SPSVD). The SPSVD recognizes faces using half the number of computations compared to the traditional SVD and is more accurate even in the presence of light variation and occlusion.

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CP9

Optimal Parameters for Neural Network Segmentation of Medical Images

We use the Kohonen self-organized map to segment tissue and organ regions in CT scans of abdominal cross-sections with unsupervised learning. We introduce a consolidation metric to evaluate the effectiveness of the segmentation. This metric allows us to evaluate optimal Kohonen operation for segmentation: optimal neighborhood size, reasonable upper bounds for training grid density, and optimal cluster counts, as well as relative performance with Haralick and Wavelet parameters.

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CP10

Repulsive Interactions in Phase Field Models of

Membrane Fusion

Phase field methods are commonly utilized when surfaces undergoing topological changes need to be tracked. Examples include fusion and fragmentation of adatom domains, immiscible liquid droplets, and lipid membrane vesicles. We extend the phase field approach by considering a repulsive interaction between interfaces that delays the onset of their fusion. Evaluation of this repulsion requires computation of a nonlocal energy term. These nonlocal interactions contribute to bending and surface tension energies associated with the interface.

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CP10

Efficient and Accurate Long-Time Simulations of Calcium Waves in a Cardiac Cell

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

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CP10

Modeling of Fluid Drop Deposition in Virtual Wells in High Throughput Screens Using Variational Principles

The movement/measuring of small amounts of fluids onto/into high density, high throughput screening wells is a source of failure for screening assays. Virtual wells offer a simpler alternative. Virtual wells manipulate small amounts of fluid by exploiting hydrophobicity and hydrophilicity of fluids with respect to virtual well surfaces. We model droplet deposition, stretching and partitioning using a set of differential equations derived from an energy functional minimizing surface area of the droplets. Impact of this work is in the discovery and lead series optimization phases of drug development.

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CP10

Dynamics of Lipid Bilayer Vesicles in Viscous Flow

The dynamics of a lipid bilayer vesicle in a Stokes flow is studied. The bending resistance of the membrane, the transport of lipids along the monolayers, and the slip between the monolayers are taken into account. Small amplitude perturbations from a spherical vesicle are considered. At leading order, a nonlinear system of equations for the dynamics of the interface and the mean lipid density is found. This system is solved numerically and solutions are presented.

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CP10

Mathematical Modeling of Fluid Flow Through a Porous Deformable Arterial Wall

We develop a mathematical model of fluid flow interactions within a deformable arterial wall. We use mixture theory to compute both the structural displacement of the solid and fluid motion. The coupled system of equations is solved numerically. We compare the mixture theory model to a hierarchy of models including simple spring models as well as elastic deformation models. The applications of the model are to understand the deformation of the wall as a function of its material properties and the relation of this deformation to the growth and rupture of aneurysms.

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CP10

Computational Estimation of Fluid Mechanical Benefits by Modifying the Shape of Artificial Vascular Grafts

Intimal hyperplasia (IH) at the distal end of artificial grafts is considered an important determinant in graft failure. We use CFD modelling to study fluid mechanical impact for various graft designs. This is motivated by the connection between IH and unhealthy hemodynamics. We focus on IH at the suture line and demonstrate benefits by the introduction of a fluid deflector that shields the suture line from unhealthily high wall shear stress.

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CP11

A Simple Model for Laser Drilling

Laser drilling is used in many industries due its advantages over conventional drilling techniques. Advantages include low heat release, consistency and accuracy. The process is quite involved and includes absorption and reflection of the beam, creation of plasma and melt ejection. The goal of this work is to show that for some regimes, simple and fast computational models can very accurately predict depth penetration, the fore most important aspect of the process. To this end, we will describe a quasi one-dimensional model and compare its prediction to experimental results.

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CP11

A Family of Composite Time Integration Algorithms for Nonlinear Dynamic Analysis

Temporal unconditional stability and high-frequency numerical dissipation are crucial for robust and long-time simulations of dynamic nonlinear structural problems involving large deformations. We present a class of new time-integration algorithms for solving 3D dynamic geometrically-nonlinear elasticity equations by integrating a second-derivative type scheme and the Newmark-(β,γ) (γ=1/2) scheme into a composite method. These algorithms are second-order accurate in time, dissipative for high frequencies, self-starting, and stable for nonlinear elastodynamic problems. These algorithms are implemented and tested together with a high-order spectral element method for spatial discretization of the 3D elasticity equations. We demonstrate the stability of the time-integration algorithms and compare their performance with existing methods for a number of 3D nonlinear elastodynamic problems involving large deformations.

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CP11

Shock Formation and Stability in Granular Avalanches

A nonlinear first order PDE derived by Gray and Thornton describes transport, mixing and segregation of particles of two different sizes in a granular avalanche. An unusual feature of the PDE is a depth-dependent coefficient representing shearing within the avalanche. Analysis of shock formation from smooth 2-D initial data is presented, together with numerical simulations. Further analysis demonstrates how shocks lose stability, forming a confined mixing zone.

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CP11

Simulation of the Potential Flow Using the Boundary Element Method with Higher Order Elements for the Control of the Underwater Vehicle

This work presents the efficient Boundary Element Method with higher order elements (BEM) to solve the potential flow problem which incorporates the dynamics of the Autonomous Underwater Vehicle (AUV). Numerical results are obtained by implementing an hydrodynamic model using the Boundary Element Method with higher order elements to compute efficiently the flow over solid body. Once the potential-flow equation is solved, Bernoulli's equation is applied to find the pressure distribution over the body. The pressure is then integrated to yield the total hydrodynamic forces and moments exerted on the vehicle. These total forces and moments cause the motions and determine the position and orientation of the vehicle. The six degrees of freedom will be determined using the unsteady forces and moments as calculated by a transient hydrodynamic solver instead of the empirical formula. This modeling approach which combines fluid flow, rigid body motion and control system within the same model will be more realistic and will improve the development of AUVs control systems. The dynamic model of the underwater vehicle in six DOF and the neural network predictive control model will be introduced and implemented to control the underwater vehicle.

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CP11

Lagrangian Coherent Structures in Biolocomotion

We present the results of numerical simulations of swimming hydromedusae, including flow analysis using Lagrangian coherent structures (LCS). LCS are a time dependent analog to stable and unstable manifolds in homogeneous dynamical systems and are useful for identifying flow structures and barriers to fluid transport. We highlight key flow structures and discuss their importance for locomotion as well as the different types of hydromedusan locomotion and how they effect propulsive performance and fluid transport.

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CP11

Stretching of (Heated) Viscous Filaments

Stretching of (heated) viscous filaments arises in many industrial processes and engineering applications. In this talk, I will describe the associated physical problem, the fluid model, analysis of the model, and numerical results. Also, a description of recent work on the analysis of other models for stretching of viscous filaments will be given.

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CP11

Saddle Point Problems in Liquid Crystal Modelling

This work studies the iterative solution of saddle-point problems in liquid crystal numerical modelling. Such problems arise whenever director models are implemented, through the use of Lagrange multipliers, or when an electric field with constant voltage is present. In particular, the combination of these two situations presents a real challenge in terms of numerical linear algebra. We will present some examples and discuss their efficient solution using appropriate preconditioned iterative methods.

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CP12

Noise-Induced Oscillations in An Actively Mode-Locked Laser

Mode-locked lasers are widely used as a means to generate ultra-short pulses with pulse-widths down to a few femtoseconds and with power up to tens of watts. There are many different types of mode-locked lasers, but they have many commonalities. We focus on an actively mode-locked laser. In particular we focus on the destabilization of the system due to noise. The effects of additive, proportional, and combined noise is considered in this presentation. Spatial noise is approximated by Hermite expansions and temporal noise is approximated via an approximation of the variance of the random variable using a fourth order Adams-Bashforth scheme. The approach is verified on a sample problem and used to explore the governing equations for a mode-locked laser. The impact of noise on additive and multiplicative terms is explored, and the inclusion of multiplicative noise directly impacts the time between pulses resulting in longer intervals between pulses.

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CP12

Plasmonic Waveguide: Mathematical Modeling and Numerical Simulations

Surface plasmons are optical waves that can propagate along a metal-dielectric interface with a subwavelength confinement. This characteristic makes them very interesting in nano-photonic applications. In order to develop them, the understanding of light propagation in plasmonic waveguides results essential. Our study is devoted to accurately compute the modes of these structures. Simulations of arbitrary geometries are addressed by a suitable implementation of a Finite Element Method with appropriate transparent boundary conditions, preventing spurious solutions.

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CP12

Positional Disorder in Photonic Crystals

Much is known about the propagation of waves through photonic crystals. Here, we consider a simple realization: scalar waves through a regular two-dimensional array of identical small circles. We are interested in the effect of random disorder: the circles remain identical, but their centers are given small random displacements. We derive asymptotic approximations which can be used to quantify the effect of positional disorder. Extension to more complicated problems seems feasible.

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CP12

Modeling Laser Mode-Locking for Generation of Multiple Pulses Per

The use of an intra-cavity Mach Zehnder interferometer (MZI) for the controlled generation of multiple pulses per roundtrip in passively mode-locked lasers is modeled and evaluated. Proper operation requires matching between the MZI differential delay and phase difference and the roundtrip time and phase slip of the surrounding laser cavity. The presence of the MZI is accounted for by introducing modifications into the usual complex Ginzburg-Landau equation that describes the mode-locked laser. Control strategies and their effect are considered.

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CP13

Non-rigid matching models based on Hellinger dis-

tance

A new model to estimate the correspondences and the non-rigid transformations between point-sets/ shapes/ images are proposed. This model utilizes an algorithm analogous to the soft-assign technique in non-rigid matching problems. This model possesses the parameterization invariance property, which enables us to match many objects, while performing principal component analysis. Besides, it also exhibits theoretical features analogous to the optimal mass transport model. Some numerical results are presented to show its effectiveness.

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CP13
Metrics Defined by Bregman Divergences

Bregman divergences are generalizations of the well known Kullback Leibler divergence. They are based on convex functions and have recently received great attention. We present a class of "squared root metrics' based on Bregman divergences. They can be regarded as natural generalization of Euclidean distance. We provide necessary and sufficient conditions for a convex function so that the square root of its associated average Bregman divergence is a metric.

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CP13
Modeling Analysis and Simulation of Ant-Based Routing and Forwarding Protocols.

Ant-based protocols provide elegant solutions to the routing and the forwarding problems of both wired computer networks and mobile wireless networks. These protocols use packets to discover new routes and reinforce efficient routes by adjusting pheromone values along links as they stochastically traverse the network. We present new nonlinear stochastic models and compare them to network simulations with high-fidelity protocol and physical layer models, Through analysis of the models, we determine design principles for appropriate parameter selection to ensure near optimality, stability or redundancy.

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CP14
Fourier Based Fast Multipole Method for the Helmholtz Equation

We present a formulation of the Helmholtz FMM using Fourier basis functions rather than spherical harmonics that accelerates some of the time-critical stages of the algorithm. With modifications to the transfer function in the precomputation stage of the FMM, the interpolation and anterpolation operators become straightforward applications of FFTs. Using Fourier analysis, constructive algorithms are derived to a priori determine an integration quadrature for a given error tolerance. Sharp error bounds are mathematically derived and verified numerically.

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CP14
Fast Interpolation Schemes Based on Sobolev-Type Norm Minimization

We present a higher order interpolation scheme with Runge Phenomenon suppression. The central idea is to find the set of interpolating polynomials, minimizing a Sobolev-type norm. The chosen norm depends on the underlying function. The scheme is easily extensible to higher dimensions and works on scattered data. Using a Golomb-Weinberger type formulation for the interpolation problem, we study the structure of the interpolating kernel and propose fast algorithms based on Fast Multipole Methods.

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CP14
A Simple Spectral Collocation Method for Hyperbolic Equations with Singular Sources

Spectral approximations of singular solutions yield the so-called Gibbs phenomenon in general. Regularizing the singular source term may reduce the Gibbs oscillations but convergence in maximum norm still does not decay. A simple spectral collocation method is developed based on the direct projection method for the approximation of the singular source. The spectral approximation of the singular source term is highly oscillatory but yields a nice solution due to a cancellation on the collocation points. Some linear and nonlinear equations are solved including the kink-impurity interactions of the sine-Gordon equations in defected media and collision equations in the particle limit. Numerical examples also include the moving singular source term, for which the spectral approximation of the singular source is obtained in the transformed coordinate.

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CP14

Approximation of a General Implicit Function

For a continuously differentiable mapping $H : R^{N+K} \to R^N$ and $x_0 \in R^N$ such that $H(x_0) = 0_N$ and the derivative (with respect to the first N variables) $\frac{\partial H}{\partial[x_1,\ldots,x_N]}(x_0)$ is of full rank, we construct an approximation to the implicit function $f : [x_{N+1}, \ldots, x_{N+K}] \to [x_1, \ldots, x_N]$ so that

$$H(f([x_{N+1}, \ldots, x_{N+K}]), x_{N+1}, \ldots, x_{N+K}) = 0_N$$

in some neighborhood of $[x_1, \ldots, x_{N+K}]_0$. The approximation is based on the use of a Radial Basis Function approximation applied to data points that lie on the pseudomanifold generated by the piecewise linear approximation to the system of equations $H(x_{N+1}, \ldots, x_{N+K}) = 0_N$. The method for generating this approximation is described and error estimates are given.

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CP14

A Interpolation-Based High-Order Meshless Scheme for Partial Differential Equations in Complex Geometry

We construct a finite difference scheme based on our multivariate interpolation scheme [Q. Wang et al. A Rational Interpolation Scheme with Super-Polynomial Rate of Convergence. CTR Annual Research Briefs. Stanford, CA]. The spacial derivatives are approximated using the derivative of the interpolant. High-order convergence is observed for wave equation on arbitrary grids with no mesh. Stability analysis and boundary conditions are also discussed.

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CP15

Integrated Variance, a Bayesian Approach

We present a Bayesian approach to estimating the integrated variance implied by option prices. In addition to option market data, we use very general prior information. A hyperprior, determined by the data, helps us to catch the skewness of the distribution of interest. The implied integrated variance implied is independent of strike prices, which simplifies the pricing of illiquid options. An example demonstrates estimating prices of variance and volatility swaps and calls.

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CP15

Comparison of Direct and Iterative Solvers for Finite-Difference GPU-Based Valuation of American Options

Modern option trading systems require highly efficient and accurate algorithms for computing theoretical values and Greeks of American options. In this presentation we consider a high-order finite-difference scheme for solving the time-dependent Black-Scholes equation for the American option. We present results for both direct and iterative solutions of the resulting banded linear system. In particular, we analyze the performance of the implemented solvers that are optimized for numerical valuation on graphics processing units (GPUs) using GPULib.

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CP15

Project Evaluation Based on Time-Reversed Lindley Equation

In competitive business environment, if you win, you could obtain huge reward from your project. However, in the most cases, you lose in the competition and the profit may not cover your investment. We need evaluate such projects of the negative expected return with occasional high return. Since the expected return is negative, net present value analysis and real option analysis will tell us that it is irratinal to invest in such projects, so it is difficult to evalutate those risky project. In this research, we will use the time-reversed Lindely formula, to describe the maximum return from the project, given that you have option to stop the project if it is not profitable in the future. Since Lindley equation is used in queueing theory to describe the waiting time process, we can use theoretical knowledges in queue theory to evaluate the return of the project. Particularly, we employ the large deviation analysis to evaluate the project with negative expected return.

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CP16

The Discontinuous Galerkin Method for Two Dimensional Hyperbolic Problems

We will investigate the superconvergence properties of the discontinuous Galerkin method applied hyperbolic problems on triangle meshes. We show that the discontinuous finite element solution is $O(h^{p+2})$ superconvergent at the Legendre points on the outflow edge for triangles having one outflow edge. For triangles having two outflow edges the finite element error is $O(h^{p+2})$ superconvergent at the end points of the inflow edge. We apply these results to construct simple, efficient and asymptotically correct *a posteriori* error estimates of the finite element error.

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CP16

High Order Mimetic Discretizations on Nonuniform Grids

Mimetic operators or summation-by-part operators (as they are sometimes called) are finite difference like approximations to differential operators that replicate symmetry properties of the continuum operators and could be thought as a discrete analogs of vector and tensor calculus. We will present an expansion of the operators to nonuniform logically rectangular grids in one and two dimensions as well as some examples.

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CP16

Accuracy and Stability of the Continuous and Discontinuous Finite Element Methods for Elastic Wave Propagation

There is currently an increasing interest in numerical seismology for the high-order Finite Element Methods to simulate the propagation of elastic waves in geophysical models. Two methods that are particularly suited for this problem are the Spectral Element and the Discontinuous Galerkin Methods. Unfortunately their accuracy and stability are not well understood. We study their stability and accuracy in terms of grid dispersion, and present analytic results for benchmark problems and realistic models.

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CP16

Finite Element Splitting Extrapolation: a Convergence Acceleration Algorithm Based on Domain Decomposition

This presentation discusses a finite element splitting extrapolation for solving PDEs. By domain decomposition, independent mesh parameters are chosen and a large scale multidimensional problem is turned into some smaller discrete subproblems which can be computed in parallel with high degree of parallelism. This method improves the accuracy with less computational complexity than Richardson extrapolation and only requires piecewise smoothness for analytic solutions. Additionally, this method is efficient for solving interfaces problems and nonlinear equations.

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CP16

An Extended Finite Element Method for Fluid Topology Optimization by Kinetic Theory

An extended finite element method(XFEM) is proposed for the topology optimization of fluids via kinetic theory approaches. The boundary condition is accurately imposed by the projected Lagrange multiplier. In the sensitivity analysis, the adjoint method is applied through numerical finite differencing and analytically derived formulation. Numerical examples are illustrated with the channels of pipebend and manifold with minimal pressure drop. As a whole, XFEM shows competitive results for topology optimization problems by kinetic theory.

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CP16

The Wkb Local Discontinuous Galerkin Method for the Simulation of Schrodinger Equation in a Resonant Tunneling Diode

We develop a multiscale local discontinuous Galerkin method to simulate the one-dimensional stationary Schrödinger-Poisson problem. The stationary Schrödinger equation is discretized by the WKB local discontinuous Galerkin (WKB-LDG) method. The WKB-LDG method we propose provides a significant reduction of both the computational cost and memory in solving the Schrödinger equation. Comparing with traditional continuous finite element Galerkin methodology, the WKB-LDG method has the advantages of the DG methods including their flexibility in *h-p* adaptivity and allowance of complete discontinuity at element interfaces. A major advantage of the WKB-LDG method is its feasibility for two-dimensional devices.

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CP17

On the Problem of Aizerman for Second-Order Systems with Multiple Delays

The paper considers the second-order differential equation with multiple delays not involving derivatives:

$$\ddot{x} + a_1\dot{x} + \phi(x) + \sum_{j=1}^{m} b_j x(t-\tau_j) = 0$$

It will be proved that for this system the Aizerman conjecture is true, i.e., the stability of (1) can be inferred from the stability of the following linear system:

$$\ddot{x} + a_1\dot{x} + ax + \sum_{j=1}^{m} b_j x(t-\tau_j) = 0$$

The proof of this result is based on the Popov stability criterion. This paper is the continuation of the one presented at the 2008 SIAM Annual Meeting in San Diego.

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CP17

Dynamics of the $1, n$ Compound Pendulum

We analyze the motion of the $1, n$ compound pendulum, that is, a pendulum system with one upper and n lower pendula. In contrast to the more well known the double pendulum, the $1, n$ pendulum exhibits an exchange of energy between the lower pendula, which can lead to bursts of over-the-top motion for one or more of the lower pendula as their energy is suddenly pumped up from a lower energy state.

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CP17

Explicit Autonomous Suspensions of Orientation Preserving Maps

We demonstrate a general method whereby an invertible, orientation preserving map M with a bounded, invariant attracting set can be suspended to a flow generated by an explicit system of autonomous differential equations. The flow is exact in an open neighborhood U of the attractor, insofar as the dynamics at the Poincaré section are exactly those of the original map acting on U.

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CP17

A Polynomial Suspension of the Henon Map

We create polynomial differential equations for a suspension of the Henon map. By globalizing the local tangent vectors to suspended periodic orbits, we are able to find approximate autonomous differential equations for the suspension. Using as few as two carefully chosen suspended periodic orbits, we are able to generate robust three dimensional attractors whose Poincare maps have very nearly the dynamics of the original map.

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CP17

Synchronization in Logistic Networks with Adaptive Competition

A general N-node network is considered for which, in absence of interactions, each node is governed by a logistic equation. Interactions among the nodes take place in the form of competition, which also includes adaptive abilities through a (short term) memory effect. As a consequence the dynamics of the network is governed by a system of NxN nonlinear ordinary differential equations depending on: the strength of competition, the adaptation characteristic time and the size of the network. Existence and stability of the equilibria are discussed analitically in full generality. Time-dependent regimes exhibit remarkable properties of synchronization both in the case of periodic oscillations and chaotic behavior, related to the existence of attractive invariant subspaces. Depending on the network size, the loss of synchronization may happen when increasing the adaptation time the invariant subspaces loose attractiveness.

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CP18

Data Compression and Comparison Using Parallel-Configured Prime Enumeration

A new algorithm is presented to compress, compare, store and regenerate long strings of data. The algorithm uti-

lizes a unique parallel decomposition that incorporates prime numbers as multipliers combined with simple modular arithmetic to manage the strings. Multiple data layers increase retrieval flexibility. Examples illustrate application to genetic haplotype data.

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CP18

Krylov Subspace Computation on Hybrid Multicore Platforms

We analyze vector orthogonalization computations for Krylov methods on hybrid multicore architectures: CPU/GPU or Cell processors. We evaluate classical and modified Gram-Schmidt processes, with or without re-orthogonalization strategies, on multiple GPUs or Cells platforms to accelerate computations. We study the quality of the basis orthogonality with respect to arithmetics of the targeted processors and analyze the Ritz eigenvectors associated to these subspaces to conclude on possible benefits of these accelerators to compute large Krylov subspaces.

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CP18

Reusable Numerical Libraries for Large-Scale Distributed Computation

Currently the majority of numerical libraries cant exploit the large number of nodes and cores which compose new distributed architectures. We propose a design of parallel/distributed numerical libraries based on a component approach. It allows the sequential and parallel code re-use while providing the optimization of the performances. Our model is based on a strict separation between the flow of control and the management of the data flow. We present its application to some existing libraries.

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CP18

Openmp and the Multi-Core Programming Challenge

Multicore chips require parallel software, but how should programmers create this software? One option is OpenMP, a shared memory programming model that lets programmers sprinkle their code with directives and smoothly evolve a serial program into a parallel program. Of course, this is an over simplification and in practice, things can be much more complicated. But even with these complications, we believe OpenMP is one of our best options for addressing the multi-core programming challenge.

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CP19

Classical and Semiclassical Molecular Dynamics Simulation of polar liquids

We will present an overview and results of our ongoing work on the simulation and computation of properties of polar liquids. Part of our work is on treecode methods aimed at speeding up the force computation for large classical polar liquid systems. We are also working on semiclassical methodology for computing the vibrational energy relaxation (VER) of polar liquids. Until now, much of the effort has been on computing the VER of non-polar liquids.

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CP19

Using Optimal Time Step Selection to Boost the Accuracy of Finite-Difference Schemes for Variable-Coefficient and Systems of Time-Dependent PDEs

An optimal choice of time step can be used to boost the order of accuracy of formally low-order finite-difference schemes for time-dependent scalar PDEs. This talk presents extensions of the technique of optimal time step selection to variable-coefficient and systems of PDEs. For variable-coefficient PDEs, higher-order accuracy is achieved by combining optimal time step selection with optimal grid choice. For systems of PDEs, a simple synchronization procedure can be used to achieve higher-order accuracy when the individual PDEs have different optimal time steps. We demonstrate the utility of these extensions by applying them to several example PDEs and explain the observed orders of convergence explained via straightforward numerical analysis arguments.

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CP19
Simple Waves Do Not Avoid Eigenvalue Crossings

Wigner and von Neumann have shown that in general one-parameter families of matrices avoid eigenvalue crossings. We are considering solutions to quasi-linear PDEs which are simple waves. We have shown that in phase space there is a sector, starting in which the simple waves are attracted to degenerate points.

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CP19
Squeezing the Most of Out Time-Parallelism for Accelerating the Solution of Time-Reversible ODEs

The Parallel-In-Time Algorithm is an iterative Newton-like method that relies on a partition of the time-domain on which the system evolution can be computed concurrently using a classical time- integrator. When the problem is time-reversible, forward and backward-in-time integrations can be carried out simultaneously for an almost doubled parallel potential. A theoretical analysis of the methodology is developed and the application to undamped structural dynamics is presented with experimental results and a practical performance assessment.

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CP19
Unbounded Solutions of the Modified Korteweg-De Vries Equation

We prove local existence and uniqueness of solutions of the focusing modified Korteweg - de Vries equation $u_t + u^2 u_x + u_{xxx} = 0$ in classes of unbounded functions that admit an asymptotic expansion at infinity in decreasing powers of x. We show that an asymptotic solution differs from a genuine solution by a smooth function that is of Schwartz class with respect to x and that solves a generalized version of the focusing mKdV equation. The latter equation is solved by discretization methods.

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CP20
Computing Generalized Langevin Equations and Generalized Fokker-Planck Equations

Many applications such as molecular dynamics lead to the solution of a system of ordinary differential equations involving a wide range of time scales. Carrying out these simulations using brute force techniques is impractical. This issue can be addressed by the Mori-Zwanzig projector formalism which allows formulating equations for reduced sets of variables. We propose new numerical and mathematical approaches for this problem. This has application in bio-molecular modeling.

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CP20
A Trust Region Method for Optimal H_2 Model Reduction

We present a trust-region approach for optimal H_2 model reduction of multiple-input/multiple-output (MIMO) linear dynamical systems. The proposed approach generates a sequence of reduced order models producing monotone improving H_2 error norms and is globally convergent to a reduced order model guaranteed to satisfy first-order optimality conditions with respect to H_2 error criteria. Unlike existing H_2 descent methods, the method does not require solving any Lyapunov equations and is both numerically stable and computationally tractable even for very large order systems. This method appears to be the first descent approach that uses Hessian information for optimal H_2 model reduction of MIMO dynamical systems.

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CP20
Morphologically Accurate Reduced Order Modeling of Spiking Neurons

Simulating active neurons with realistic morphologies and synaptic inputs requires the solution of large systems of nonlinear ordinary differential equations. Using model re-

duction techniques of proper orthogonal decomposition and an empirical interpolation method, we recover the complete neuronal voltage dynamics using a system of dimension nearly two orders of magnitude smaller than the original and that simulates one order of magnitude faster, without sacrificing the spatially-distributed input structure.

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CP20

Mesoscopic Dynamics of Large Ode Systems

The main question addressed in the talk is as follows. How to produce computationally feasible and practically useful simulations of large ODE systems? A typical size of such systems is 10^7 unknowns or more. In a typical application, the actual solutions are rarely needed. Instead, one might be interested in simulating evolution of certain functionals of solutions, called observables. The number of such functionals can be small (1-10). We present some new ideas on how to obtain a closed system governing evolution of observables, starting from an ODE system. The proposed approach is based on space-time averaging and concentration inequalities from probability theory.

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CP21

Stochastic Semidefinite Programming

Stochastic Linear Programs (SLP's) and semidefinite programs (SDP's) are two classes of useful and well-studied optimization problems. Stochastic semidefinite programs (SSDP's) are a class of optimization problems introduced by the first and the second authors extending SLP's and SDP's. We present a summary of our recent results on SSDP's.

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CP21

A Stochastic Optimization Problem Modeling Seasonal Plant Reproduction and Survival

We will present a stochastic optimization problem in ecology based on the survival and reproductive strategies of a plant species in a risky environment. The model maximizes the expected overall plant biomass production at the end of a season subject to growth governed by a stochastic differential equation. We will present analytic solutions for this model, simulation data, and implications for evolutionary strategies. We will also discuss parallels with a financial problem in optimizing wealth.

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CP21

.Optimal Control of a Biological Waste Cleaning Plant.

A mathematical model of a waste cleaning water plant is created and investigated. The model is described by a nonlinear system of two differential equations with one bounded control. An optimal control problem of minimizing concentration of contaminated water with the terminal functional is stated and solved. Optimal solution is obtained analytically. Possible applications are discussed.

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CP21

Robust Optimization of Discretized Dynamical Systems with Stability Constraints

We present an optimization method for nonlinear discrete-time systems particularly suited for engineering problems, as it can cope with critical dynamical boundaries (e.g. stability boundaries) for uncertain models. In typical applications, technical systems are optimized economically, while guaranteeing a user-specified parametric distance to critical points (e.g. bifurcations). Attention must be paid to preserving critical boundaries when discrete-time models result from sampling continuous-time models. The method is illustrated with a fermentation process.

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CP21

Analyzing Functions of Fuzzy Intervals Via Optimization and Gradual Numbers

Many applications require evaluation of functions of uncertain variables (e.g. measurements obtained with imprecise instruments.) Propagating this uncertainty through a function often results in an overestimation of the error. We propose a method for exact evaluation of differentiable or convex functions when the variables uncertainty is represented by a fuzzy interval. We incorporate recently introduced gradual numbers with well-known optimization techniques to improve over existing techniques with increased efficiency and closed form outputs.

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CP22

Least-Squares Finite Element Methods for 4 to 1 Planar Contraction Flow of Viscoelastic Fluid

The goal of this work is to implement least-squares finite element methods for equations governing viscoelastic flows occurring in polymer processing. Model problem considered is the 4 to 1 contraction flow problem. Major difficulties include corner singularities, and loss of convergence for high values of the Deborah number. To resolve these, a mesh redistribution algorithm based on a nonlinear weighted least-squares finite element method will be developed. Numerical results of convergent meshes will be presented for the model problem.

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CP22

Martin Type "Differential" Approach: An "Algebraic" Burnat Type Classifying Characterization

Some significant contrasts and consonances are identified in a parallel between two essential gasdynamic versions [unsteady one-dimensional and, respectively, supersonic steady two-dimensional] of a Martin type "differential" approach [associated with a Monge-Ampère type representation]. The facts of this parallel are then classified with some "algebraic" arguments of a Burnat type [centered on a duality connection between the hodographic character and the physical character]. Some applications are considered concerning the Martin geometrical linearization.

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CP22

A Riemann Solver for Semirelativistic Magnetohydrodynamics: A Preliminary Report

We present a method based on the multi-state HLLD (Harten-Lax-van Leer-Discontinuity) nonlinear Riemann solver for semirelativistic magnetohydrodynamics. Although plasma may have a nonrelativistic speed, with a strong magnetic field and a sufficiently low plasma density, the Alfvén speed, proportional to the magnitude of the magnetic field and inversely proportional to the square root of the density, may be a significant fraction of the speed of light, requiring semirelativistic treatment.

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CP22

Multiscale Simulation of Fast Magnetic Reconnection

We present discontinuous Galerkin simulations of fast magnetic reconnection in nearly collisionless plasma and study the dependence of magnetic reconnection on diffusive modeling parameters. We focus on the GEM magnetic reconnection problem. We use two-fluid physics for the microscale (reconnection) region and magnetohydrodynamics for the majority of the domain.

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CP22

Greens Function Technique for Radiation Transport in 3D

Future missions in Earths orbit, to near-Earth space, the Moon and Mars will expose crewmembers to the space radiation environment for extended periods of time. The intensity of the ions in this environment must therefore be reduced while holding secondary radiation to a minimum within the spacecraft interior where the astronauts spend most of their time. A common code to validate laboratory and space measurements is tested using Greens functions as the solution to the Boltzmann Transport Equation.

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CP22

Phase Transition Approach to Detecting Singularities of Partial Differential Equations

We present a mesh refinement algorithm for detecting singularities of time-dependent partial differential equations. The main idea behind the algorithm is to treat the occurrence of singularities of time-dependent partial differential equations as phase transitions. We show how the mesh refinement algorithm can be used to calculate the blow-up rate as we approach the singularity.

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CP23

Mathematical and Numerical Models for the Char-

acterization of Cerebral Aneurysm Walls

A multi-mechanism model was introduced by Wulandana and Robertson, in order to model the onset and early growth of cerebral aneurysms. They are saccular dilations of cerebral arteries. The model is based on the behavior of collagen and elastin, that are passive components of arterial wall. They enter the model a separate mechanisms with different material response and unloaded configurations. We extended the multi-mechanism model in order to implement it in a C++ library. Simplified geometries as well as real geometrical models obtained by CT scans, have been used in the numerical simulations.

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CP23

Application of Control Theory in Modeling of Brain Cancer

In this paper a mathematical model is presented that describes the concentration of tumor cells of the brain. The treatment of the brain cancer is interpreted as an optimal control problem. Evolution of the disease is characterized by a parabolic partial differential equation that describes the growth of a tumor brain. While biomedical research concentrates on the development of new drugs and experimental and clinical determinations of their treatment schedules, the analysis of mathematical models can assist in testing various treatment strategies and searching for optimal ones. Using the considered mathematical model, we try to solve some medical problems in brain canser.

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CP23

On Some Stochastic Dynamical Systems and Cancer

Different models of tumer growth are considered. Some mathematical methods are developed to analyze the dynamics of mutations enabling cells in cancer patients to metastize. The mathematical models consist of some stochastic dynamical systems describing tumer cells and immune effectors. It is also considered a method to contrast the ideal outcomes of some treatments. The results of the considered model predict continuous under which some suitable treatment can be successful in returning an aggressive tumer to its passive, non-immune evading state. The principle goal of this paper is to find ways to treatment the cancer tumer before they can reach an advanced stage development.

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CP23

Treecode-Accelerated Poisson-Boltzmann (PB) Solver for Biomolecular Simulation

A treecode-accelerated PB solver, which combines both efficiency and accuracy, was developed using a boundary integral formulation and collocation method. This boundary integral frame addressed numerical difficulties arising from geometric surface complexity, singular point charges, an unbounded computational domain, and discontinuous dielectric function and electric field. The associated treecode has several appealing features such as low memory requirement, simple implementation, and adaptability to complex geometry and singular integrals. Benchmark tests have been carried through.

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CP23

A Mathematical Model of Glioma Invasion

Glioblastoma is the most common primary tumor of the brain, and has a dismal prognosis, with a mean survival of around 1 year from diagnosis. Invasion of surrounding brain tissue is one of the main hallmarks of gliomas, and is a major reason for treatment failure, because tumor cells remaining after surgical resection cause tumor recurrence. Although tumors show preferred invasion routes in the brain, at present it is not possible to predict patterns of invasion and recurrence for a given tumor. Variations are seen in the numbers of invading cells, and in the extent and patterns of migration. Cells can migrate diffusely and can also be seen as clusters of cells distinct from the main tumor mass. This kind of clustering is also evident in vitro using 3-D spheroid models of glioma invasion. This has been reported for U87 cells stably expressing the constitutively active EGFRVIII mutant receptor, often seen expressed in glioblastoma. In this case the cells migrate as clusters rather than as single cells migrating in a radial pattern seen in control wild type U87 cells. Several models have been suggested to explain the different modes of migration, but none of them, so far, has explored the important role of cell-cell adhesion. We develops a mathematical model which includes the role of adhesion and provides an explanation for the various patterns of cell migration. It is shown that, depending on critical parameters, the migration patterns exhibit a gradual shift from branching to dispersion, as has been reported experimentally.

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CP23

Modeling Intercellular MAPK Signaling in An Epithelial Wound Healing Assay

Experiments in epithelial wound healing have demonstrated the necessity of MAPK activation for coordinated cell movement after damage. We develop a mechanistic model that produces the observed behavior by exploring the ligand/receptor coupling in the activation of the MAPK cascade. We study the bi-stability of the model in connection with the bi-stability of the MAPK cascade. In particular, we look for traveling wave solutions of the model and their properties under various regimes.

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CP24

Convergence Improvement of Non-Overlapping Domain Decomposition Method: Helmholtz Equation

A new non-overlapping domain decomposition algorithm for the Helmholtz equation is introduced. Based on an adequate approximation of the Stecklov-Poincaré operator, we derive transmission conditions that provide a rapidly-convergent iterative procedure. Numerical simulations are presented in the context of a boundary and finite element methods coupling algorithm.

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CP24

Random Sampling High Dimensional Model Representation Via Fluctuation Free Integration

High dimensional model representation (HDMR) (Sobol, Rabitz, Demiralp) is composed of components in ascending multivariance starting from a constant term followed by univariate and high variate terms. These components are uniquely determined by multiple integration. Generally, Monte Carlo methods or Generalized HDMR is used for integration. This work focuses on the fluctuation free integration based on the approximation of a function's matrix representation by the image of the independent variable matrix representations under the same function.

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CP24

Randomization of Forcing in Large Systems of Pde for Improvement of Energy Estimates

In many physical applications, one is interested in computing an energy associated with a system of linear PDE driven by localized forcing. For large systems, where direct computation is inhibitive, we study its related stochastic PDE, and use a change of basis method to estimate the energy to high accuracy, and with significant reduction in computational cost. We establish vast improvements for simple convection-diffusion equations, and also good improvements for the 2D wave equation.

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CP24

The Application of the Fast Fourier Transform to Jacobi Polynomial Expansions

We observe that the connection coefficient relations transforming modal coefficients of one Jacobi Polynomial class to the modal coefficients of certain other classes are sparse. When one of the classes corresponds to the Chebyshev case, the Fast Fourier Transform can be used to compute modal coefficients for Jacobi Polynomial expansions of class (α, β) in $O(NlogN)$ time when 2α and 2β are both odd integers. We present numerical results to illustrate efficiency and accuracy.

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CP24

A Projection Method for Nonlinear Eigenvalue Problems Based on Complex Contour Integration

We present an algorithm that can compute all the eigenvalues of the nonlinear eigenvalue problem $A(z)\mathbf{x} = 0$ in a closed curve on the complex plane. Our algorithm is an extension of Sakurai and Sugiuras algorithm for the generalized linear eigenvalue problem. Interestingly, the computational work does not increase due to the existence of nonlinearity. In this talk, we present the theory behind our algorithm and give numerical results that illustrate the accuracy of our algorithm.

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CP25

Optimal Power Generation under Routine and Extreme Electric Grid Variability

Domestic productivity and security rely critically on the stability of the electric power grid. Routine performance deviations (due to normal reliability-based component failure) and unexpected outages (caused by less likely disruptions with greater impact), both affect the grids ability to meet power demand within operational constraints. This talk will demonstrate large-scale optimization of generation profiles to maximize load served, as predicted by steady-state AC power flow models under both classes of interruption.

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CP25

General Order Finite Difference Schemes for Electromagnetic Wave Propagation in Dispersive Media

We present and analyze temporally and spatially staggered second order accurate in time and 2n- (i.e., even) order accurate in space finite difference schemes for electromagnetic wave propagation in Debye and Lorentz dispersive media. The stability and dispersion analyses of these schemes leads to a general formula for the stability polynomials and numerical dispersion relations for the 2n case. We also compare these schemes to the well known Yee scheme and validate our results via numerical examples.

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CP25

Stability and Error Analysis of the Cole-Cole Dielectric Model

We present an analysis of the numerical stability and accuracy for a numerical scheme to solve a fractional hyperbolic PDE system which finds application in the computation of electromagnetic pulses propagating in dispersive dielectrics whose permittivity is represented in the frequency-domain by the Cole-Cole model $\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{(1+(i\omega\tau)^\alpha}$, $\alpha \in (0, 1)$. Validation of our analysis using numerical solutions will also be presented.

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CP25

Modeling Dispersive Mechanisms Using Distributions of Dielectric Parameters

The Cole-Cole model is known to accurately describe the dielectric response of a dispersive material over a wide range of frequencies. The model, however, does not lend itself easily to time domain simulation methods such as the Finite Difference Time Domain (FDTD) method, as it involves the approximation of fractional-order derivatives. Simulators have instead often used the physics-based Debye model (of which the Cole-Cole model is a heuristic generalization). However, this is an over-simplification of reality and thus simulations do not match data. In this work, we seek to reconcile the difficulty of implementing the Cole-Cole model by presenting an approximation of dispersive mechanisms using distributions of parameters within the Debye model.

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CP25

A Spectral Time-Domain Method for Computational Electrodynamics

This talk presents an alternative approach to the time-dependent Maxwell's equations, based on Krylov subspace spectral (KSS) methods. For other time-dependent PDE, these explicit methods have demonstrated high-order accuracy, as well as stability characteristic of implicit methods. KSS methods compute Fourier coefficients of the solution using techniques developed by Golub and Meurant for approximating elements of functions of matrices. We generalize them to coupled systems of equations, and discuss the implementation of appropriate boundary conditions.

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CP25

Overlapping Yee FDTD Method on Nonorthogonal Grids

We propose a new overlapping Yee (OY) method for solving time-domain Maxwell's equations on non-orthogonal grids. The proposed method is a direct extension of the Finite-Difference Time-Domain (FDTD) method to irregular grids. A key advantage of the OY method over other non-orthogonal FDTD algorithms is that it overcomes the late-time instability problem. Numerical examples are presented to illustrate the accuracy, stability, convergence and efficiency of the OY method.

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CP26

Multiple Scale Parabolic Equation Solutions to Seismo-Acoustic Problems

Improving the capabilities and accuracy of the elastic parabolic equation method in underwater acoustics has been an active area of research. As the shear wave speed approaches zero, the governing system becomes singular and fine grid spacing (not necessary in the water) is needed to capture subtle effects of the field. A dual grid solution and corresponding interface conditions will be described. Applications will be discussed for rough surface scattering and underwater communications.

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CP26

Gabor Operators for Pdes in Seismic Imaging

We characterize the mathematical properties of Gabor transforms and Gabor multipliers, which form an important toolset in seismic data processing techniques incorporating nonstationarity. Seismic imaging occurs in the context of inhomogeneous, anisotropic media, and mathematical modeling of the physical propagation of waves must take into account the local and global variations of parameters that characterize physical properties of the geology. Gabor techniques are an extension of the Fourier methods applied to localized signals, allowing numerical PDE models of physical material with inhomogeneities.

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CP26

Low-Reflection Local Space-Time Mesh Refinement for Elastodynamics

Efficient finite-difference techniques based on local mesh refinement in time and space is proposed and implemented for parallel 3D computations. Parallel version is based on Domain Decomposition performed for both coarse and fine grids and use of MPI library. The approach is destined for direct simulation of seismic waves for multiscale elastic media (e.g., carbonate reservoirs). The main attention is paid to stability analysis and estimation of artificial numerical reflection at interface of two grids.

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CP26

Finite Element Approximation of Coupled Seismic and Electromagnetic Waves in Gas Hydrate-Bearing Sediments

This work presents a numerical model to simulate the physical phenomena in which there is conversion between electromagnetic and kinetic energy. The electroseismic equations linking the diffusive electromagnetic and seismic wavefields are solved using the finite element method. The subsurface is modeled as a 2D fluid-saturated layered porous medium under transverse electric (TE) and transverse-magnetic (TM) modes. The numerical examples illustrate the capabilities of the procedure to detect gas hidrate bearing sediments beneath permafrost areas.

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CP26

Boundedness and Unboundedness for Elliptic Solutions in a Highly Heterogeneous Porous Medium

The medium considered consists of a connected high permeability sub-region and a disconnected matrix block subregion with low permeability. Let ϵ denote the size ratio of one matrix block to the whole domain and let the permeability ratio of the matrix block region to the connected region be of the order ϵ^2. In the connected region, uniform L^p estimate of the first order derivative and uniform Lipschitz estimate in ϵ of the elliptic solutions can be derived. We also give some examples to show L^p estimate of second order derivative and Holder gradient estimate of elliptic solutions in the medium can not be bounded uniformly in ϵ.

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CP27

A Viscoelastic Timoshenko Beam with Coulomb's Law of Friction

In this work, we consider dynamic frictional contact of a viscoelastic Timoshenko beam with Coulombs law, where its left is clamped and its right end is free. The beam is assumed to be deformed both horizontally and vertically, satisfying two contact conditions on the right end. One is the Signorini contact condition and the other is the Coulomb dry friction law. The existence of solutions is shown. Energy balance is investigated, involving frictional effects.

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CP27

Oscillatory Behavior of a Spatial Soliton in a Power Law Medium

We have investigated the trapped and oscillatory behavior of spatial solitons in a waveguide constituted by a medium with a transverse triangular index profile and has a power law dependence on intensity. Dynamics of such solitons are analyzed using the equivalent particle principle. Applying this principle to the perturbed Nonlinear Schrodinger Equation with power law, expressions for acceleration, spatial frequency, spatial period and other variables for a spatial soliton are derived. Expression of the acceleration is bounded in some cases resulting in an oscillatory behavior or a swing effect of the spatial soliton. Furthermore, the dynamics of the solitons are simulated numerically and good agreements are obtained between analysis and numerical results. Applications of the oscillatory behavior in optical devices are demonstrated.

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CP27

A Mathematical Model for the Diffusion Process in a Binary Mixture of Chemical Species

A mathematical model for the diffusion process which is especially for a binary mixture of chemical species is designed here. Consider the initial condition for t = 0, then solve the mathematical model for this condition and finally get the solution of this model. The solution is then explained through some proportional graphs in the different cases by considering some quantities as constant whereas other may vary with a fixed variation. While drawing graphs the different constant values of diffusion coefficients were taken, which show a variation of concentration with respect to time with a specific reaction rate, it also conclude that how concentration depends upon the values of different parameters included in the solution.

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MS0

Parallel MATLAB for Multicore and Multinode Computers

Abstract unavailable at time of publication.

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MS1

Adaptive Algebraic Multigrid in Lattice QCD Computations

Operators arising in lattice quantum-chromodynamics (LQCD) simulations pose various challenges to current solvers. For physically interesting configurations the performance of Krylov-subspace methods deteriorates quickly which fueled the search for preconditioners. Due to the nature of the background SU(n) gauge field classical algebraic multigrid (AMG) fails that task, but by introduction of adaptive techniques and generalization of AMG principles we were able to overcome some of the immanent challenges with our Bootstrap approach.

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MS1

Adaptive Algebraic Multigrid for the Schwinger Model of Quantum Electrodynamics

The Schwinger Model of quantum electrodynamics (QED) describes the interaction between electrons and photons. Numerical simulations of the theory require repeated solution of the two-dimensional Dirac equation. We consider two discretizations of the continuum operator based on least-squares finite elements. The resulting linear systems are Laplacian-like in structure, but contain random complex entries introduced by a background gauge field. We explore the use of adaptive algebraic multigrid as a preconditioner for the solution process.

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MS1

Adaptive Algebraic Multigrid for Nearly Singular Matrices

Multigrid solution of highly disordered nearly singular matrices is complicated by the separate difficulties introduced by these two aspects. Efficient solution of nearly singular matrices is often possible, when interpolation is built to fit known near-null space modes with high accuracy. In this talk, we consider the case of highly disordered matrices, such as those that arise in lattice quantum chromodynamics, where the near-null modes cannot be easily expressed in closed form.

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MS1

Adaptive Algebraic Smoothers

This talk will present a new method of adaptively constructing smoothers based on Local Sensitivity Analysis (LSA) for multigrid methods. Given a linear system, $Ax = b$, LSA is used to identify blocks of the matrix, A, which are "strongly connected' in a sense similar to the traditional measure of strength in algebraic multigrid methods. Block iterative Gauss-Seidel or Jacobi methods can then be constructed based on the identified blocks. The size of the blocks can be varied adaptively allowing for the construction of a class of block iterative algebraic smoothers. Results will be presented for both constant and variable coefficient elliptic problems, systems arising from both scalar and coupled system PDEs, as well as linear systems not arising from PDEs. The simplicity of the method will allow it to be easily incorporated into existing multigrid codes while providing a powerful tool for adaptively constructing smoothers tuned to the problem.

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MS2

Stochastic Online Optimization of Integrated Energy Systems

In this work, we establish an on-line optimization framework to exploit detailed weather forecast information in the operation of integrated energy systems. We first discuss how the use of traditional *reactive* operation strategies that neglect the future evolution of the ambient conditions can result into high operating costs. To overcome this problem, we introduce a supervisory dynamic optimization strategy that can lead to more *proactive* and cost-effective operations. The strategy is based on the solution of a receding-horizon stochastic dynamic optimization problem. This permits the incorporation of economic objectives, statistical forecast information, and operational constraints in a systematic manner. To obtain the weather forecast information, we employ a state-of-the-art forecasting model initialized with real meteorological data. The statistical ambient information is obtained from a set of realizations generated by the weather model executed in an operational setting. We present proof-of-concept simulation studies to demonstrate that the proposed framework can lead to significant savings in operating costs

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MS2

Designing the Smart Grid

Abstract unavailable at time of publication.

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MS2

A Linear Complemetarity System Model for Continuous-Time Single Bottleneck Traffic Flows

This talk formally introduces a linear complementarity system (LCS) formulation for a continuous-time, multi-user class, dynamic user equilibrium (DUE) model for the determination of trip timing decisions in a simplified single bottleneck model. Existence of solution to the model is demonstrated by a constructive time-stepping method whose convergence is rigorously analyzed. The solvability of the time-discretized subproblems by Lemke's algorithm is also established.

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MS2

The Manipulation of Carbon Emission Programs by Foreign Oil Producers

Abstract unavailable at time of publication.

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MS3

A Data-based Distribution Function for Floc Fragmentation in Linear Flow

Fragmentation of bacterial aggregates is not well understood, and yet is vital to understanding the overall evolution of aggregates in the bloodstream. In order to model this behavior, we need to understand the distribution of floc sizes post-fragmentation. Using three dimensional position data taken from multiple laboratory specimens, we determine the most likely breakage locations and analyze the stress induced by the flow. We then use the resulting data to construct a fragmentation distribution kernel which is compared to current distribution kernels in use.

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MS3

Persister Distribution in a Two-dimensional Model of a Dynamic Biofilm

Several tolerance mechanisms have been introduced to explain how bacterial biofilms are protected from disinfection. One mechanism describes the transition between two sub-populations of bacteria, one of which consumes nutrients, divides and is susceptible to antimicrobial agents and the other is consists of dormant bacteria that are insensitive to treatments. It has been shown that the presence of this persister sub-population can explain experimental observations of bacterial tolerance, at least in simplified domains. This investigation describes the development of a two-dimensional model of an established biofilm immersed in a flowing bulk fluid, where the biofilm influences the fluid dynamics and the fluid flow can deform the biofilm. We introduce several extensions to this model including the reaction between the biofilm and the antimicrobial, bacterial and EPS production and persister dynamics. The model and numerical methods are based on the boundary integral method (BIM) but requires an extension to the standard formulation to account for the production of mass within the biofilm. Our simulations indicate that many results from batch culture models carry over to the extended spatial domain. In particular, alternating dosing can eventually eliminate the bacteria but on a time scale that is much longer than in batch culture. We also predict that there is a heterogeneous distribution of persister cells that depends on the initial geometry of the biofilm and the dosing protocol.

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MS3

Towards An Integrated View of the Host-Biofilm Interface During Infection

Recognizing that bacteria which cause human disease often do so in biofilm form could significantly change the treatment of infectious diseases. Simple improvements include important modifications to standard drug therapies that anticipate the antimicrobial resistance induced by the biofilm lifestyle. In the longer term, better understanding promises more exotic strategies that might exploit the host-biofilm interface mechanically or immunologically. These latter approaches will require making headway in new areas of biofilm theory including models that incorporate the entire bacterial biomass present during infection (i.e., a biofilm and all of the multi- and single-cellular debris that it sheds) and the host immune systems experience of an infecting biofilm (such as penetration into biofilms by defensive molecules and cells and diffusion out of biofilms by elaborated humoral mediators of inflammation). This presentation will pose some questions from an immunologist about unanswered but math-amenable features of the host-biofilm interface, providing motivation for subsequent talks in the minisymposium.

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MS3

Phase-Field Models for Biofilm Growth and Biofilm-Flow Interaction

We derive a set of phase field models for biofilms using the one-fluid two-component formulation. The biofilm is assumed an incompressible continuum. The dynamics of the biofilm is governed by a modified Cahn-Hilliard equation. Numerical simulations are carried out and biofilm growth, expansion, streaming, rippling, and detachment in shear cells are captured. Viscoelastic properties of the biofilm is investigated as well.

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MS4

Emerging Research Challenges in Cyber Security

The ever-changing threats of cyber security raise a number of mathematical challenges. An overview of cyber security issues will be provided to identify areas where mathematical approaches are needed to explore strategies for understanding complicated behavior and to develop innovative solutions for addressing different threats.

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MS4

Structure and Dynamics of Cybersecurity Networks

The mathematical constructs of graph theory provide a foundation for examining network structure and dynamics.

I will discuss recent advances in the analysis of structured networks and the problem of network interdiction.

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MS4

Mathematical Underpinnings of Insider Threat Diagnostics and Prognostics

Insiders, those within or closely related to an organization, pose the greatest risk to an organizations information infrastructure. Diagnostics and prognostics of insider threats are perhaps the most difficult tasks, since the perpetrators are given authorized access privileges. Most existing threat mitigation systems address the threats that parties external to an organization pose to its information systems. Yet, little research has striven to mitigate threats that malicious or uninformed insiders may introduce. In this talk, we will present taxonomy of insider threat mitigation problems. For a few core categories in the taxonomy, we will provide mathematical formulations used to describe these problems, survey state-of-the-art approaches to address them, and discuss what we see as some of the key mathematical challenges in insider threat diagnostics and prognostics.

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MS4

Statistical Characterization and Detection for Authentication Data

We discuss statistical data analysis methods to detect abuse of network authentication mechanisms. Resources on an intranet typically require authentication by an individual user or client computer. For example, a network storage device can be mounted only after providing credentials that permit access to the information. Authentication logs are files that record these transactions. We present methods to discover chains of suspicious authentication records that suggest a user has gained unauthorized access to a network resource.

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MS5

A Hybrid Method for Coulomb Collisions in a Plasma

Simulation of Coulomb collisions in a plasma can be significant for problems of interest to fusion plasmas and other applications, but can be intractable for small Knudsen number. We propose a hybrid method that combines a continuum approach based on magneto-hydrodynamics, with a particle approach based on the Takazuka-Abe and Nanbu algorithms. This method uses a mixed representation of the particle distribution function as a combination of an analytic part and a particle part.

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MS5

RG and the Bump on Tail Instability

In this work we consider the application of temporal renormalization group methods to derive a two-fluid reduction for the classic problem of the bump on tail instability of plasma physics. The goal is to obtain asymptotic reductions and an associated efficient numerical method for simulating the weak interaction of the bi-maxwellan system. We also present specific metrics for determining when the two-fluid reduction is no-longer valid.

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MS5

Considerations for Hybrid Methods for Coulomb Collisions in a Plasma

The difficulty of simulating Coulomb collisions in a plasma at moderately (but not asymptotically) small Knudsen number has motivated the development of hybrid kinetic algorithms that couple fluid and particle methods. In the work of Caflisch et. al. [presented in this session], the non-Maxwellian part of the distribution function is chosen to be positive definite, and the collision implementation uses binary pairing of particles to achieve the correct conservation properties. An alternative is the "delta-f" method in which the non-Maxwellian part of the distribution is chosen to be orthogonal to the Maxwellian portion, and the collisional conservation laws are achieved through a collision-field algorithm. We will compare the resulting equations, methods, and implementation issues for evolving the Maxwellian and particle components in the two classes of algorithm. Comparisons will also be made through application examples.

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MS5
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MS6
Adaptive Waveform Design

Abstract unavailable at time of publication.

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MS6
Waveforms Considerations for Weather Radars and Applications

A major emphasis on weather radars is the quantitative estimation of the precipitation content for surveillance, forecasting and hydrological applications. Waveform design and coding for weather radars present some interesting challenges that are different compared to hard targets. Waveforms using time and phase coding are used to address problems such as range-velocity ambiguity, sensitivity enhancement for low peak-power transmitters and measurement of complete backscattering covariance matrix.

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MS6
Waveforms Considerations for Weather Radars and Applications

A major emphasis on weather radars is the quantitative estimation of the precipitation content for surveillance, forecasting and hydrological applications. Waveform design and coding for weather radars present some interesting challenges that are different compared to hard targets. Waveforms using time and phase coding are used to address problems such as range-velocity ambiguity, sensitivity enhancement for low peak-power transmitters and measurement of complete backscattering covariance matrix.

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MS6
The Quest to Optimize PSL and Merit Factor of Binary Sequences

A *binary sequence* is an n-tuple X with entries ± 1. *Autocorrelations* of X are dot products measuring resemblance between X and a shifted version of X. Two measures of autocorrelations' "nearness to zero" are the *merit factor* and *PSL*, essentially the sum of the autocorrelations' squares and the largest modulus of an autocorrelation respectively. We discuss analytic and probabilistic aspects of finding the optimum merit factor or PSL among binary sequences of given length.

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MS7
The (in)stability of Stationary Periodic Solutions of Integrable Equations

The stability of the soliton solutions of integrable equations has been well studied. Only recently have their periodic counterparts received similar attention. In this talk I will describe a general method to investigate the spectral, linear, and orbital stability of the stationary periodic solutions of integrable equations. This is joint work with Nate Bottman, Michael Nivala, and Todd Kapitula.

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MS7
Symbolic Computation of Lax Pairs of Nonlinear Partial Difference Equations

A partial difference equation is a fully discretized version of a partial differential equation. Based on work by Nijhoff, Bobenko and Suris, an algorithm will be shown to compute Lax pairs of completely integrable nonlinear partial difference equations in 2D. A Mathematica package will be presented that automatically computes Lax pairs of lattice versions of the potential Korteweg-de Vries (KdV) equation, the modified KdV and sine-Gordon equations, and lattices derived by Adler, Bobenko, and Suris.

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MS7
Stability Analysis of Persistent Periodic Solutions to a Complex Ginzburg-Landau Perturbation of the NLS Equation

It was shown by Cruz-Pacheco, Levermore, and Luce in 2004 that a certain class of periodic solutions to the nonlinear Schrodinger equation (NLS) persist when the

NLS is subject to a perturbation leading to the Complex Ginzburg-Landau (CGL) equation. In this presentation, I will show how one can use methods coming from integrability theory together with the Evans function to study the spectral stability of these persisting solutions. In particular, I will show that the solutions of NLS are spectrally stable with respect to periodic perturbations. However, the solutions can become unstable when the NLS equation is perturbed to the CGL equation.

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MS7

Discrete Integrable Systems and Their Applications

Discrete integrable systems have received much attention recently because of many applications to numerical method of nonlinear waves, computer visualization, numerical algorithms and so on. The talk will address discrete integrable systems related to a class of nonlinear wave equations including the Camassa-Holm equation. The focus is on the application of discrete integrable systems to numerical computations of nonlinear wave equations. It will be shown that discrete integrable systems provide very accurate numerical schemes.

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MS8

A New Generation of Adaptive Smooth Aggregation

We present an improved adaptive smoothed aggregation method. The new method retains favorable properties of the original incarnation, while eliminating several of its deficiencies. Numerical examples confirming improved behavior will be presented.

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MS8

Multiscale Eigensolver for 2D Differential Operators

A new multigrid solver for finding many eigenfunctions of PDEs is discussed along with some numerical results and future work. The solver employs multiscale approach that allows an accurate representation of the finest problem by an larger set of increasingly smaller problems as the solver proceeds to the coarsest grid. The algorithm is built in an adaptive algebraic framework, using Brandt's least squares method for building prolongation operators.

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MS8

An Algebraic Multigrid Method for Markov Chains

An algebraic multigrid (AMG) method is presented for the calculation of the stationary probability vector of an irreducible Markov chain. We propose a modified AMG interpolation formula, which produces a nonnegative interpolation operator with unit row sums. It is shown how the adoption of a lumping technique maintains the irreducible singular M-matrix character of the coarse-level operators on all levels. Together, these properties are sufficient to establish the well-posedness of our algorithm. Numerical results show how our method leads to nearly optimal multigrid efficiency for a representative set of test problems.

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MS8

Towards Adaptive Smoothed Aggregation Multigrid for Nonsymmetric Problems

Smoothed aggregation (SA) applied to nonsymmetric systems, $A\mathbf{x} = \mathbf{b}$, lacks a minimization principle in coarse-grid correction. Consider applying SA to symmetric positive definite (SPD) matrices, $\sqrt{A^tA}$ or $\sqrt{AA^t}$, which are full. It is not computationally efficient to use these matrices directly to form coarse-grid corrections. The proposed approach efficiently approximates these corrections using SA adaptively to approximate right and left singular vectors of A.

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MS9

The Double Life of a Program Manager and Researcher: A Balancing Act

Being a technical program manager for a funding agency while maintaining a personal research program is a lesson in balancing priorities and responsibilities. In this talk, I will draw from my own experience as a program manager for the Air Force Scientific Research (AFOSR) and an academic to emphasize the importance of maintaining this balance in order to achieve excellence in both arenas.

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MS9

Panel Discussion

This discussion section will be provide time for questions relating to academic and industrial opportunities that the speakers will address.

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MS9

The Two-Body Problem and Pre-Tenure Twins

My spouse and I have been living the "two-body problem" for a number of years. The dual-career balance has occasionally required some creativity as have other aspects of life balance such as finding time for non-math fun. Our well-honed balancing act is taking on a new dimension – our twins just arrived ten weeks early! We both elected against leaves of absence, and are juggling babies, teaching, and research, all while on the tenure track.

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MS9

Teaching, Research, and Family: Who Has the Time?

In today's academic climate, teaching and research performance expectations in colleges and universities across the country seem to ratchet ever higher. While most academics now face heightened job performance requirements, women professors, in particular, are statistically more likely to be confronted with the additional challenge of shouldering significant responsibility for family care and management. In this talk, we will discuss some coping mechanisms that can be of help in successfully navigating the path toward balancing both career and family obligations.

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MS10

Biofilm as a Physiologically Structured Fluid

We discuss a modeling and simulation approach using PDE's where cell-level processes are incorporated into a macroscale description of a biofilm using so-called structured variables.

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MS10

Fragmentation and Aggregation of Bacterial Emboli

Klebsiella pneumoniae is one of the most common causes of intravascular catheter infections, potentially leading to life-threatening bacteremia. These bloodstream infections dramatically increase the mortality of illnesses and often serve as an engine for sepsis. Our current model for the dynamics of the size-structured population of aggregates in a hydrodynamic system is based on the Smoluchowski coagulation equations. In this talk, I will discuss the progress of several investigations into properties of our model equations. In particular, I will focus on a) accurate characterization of the fractal properties for the aggregates, b) a differential geometry approach to fragmentation modeling, and (time permitting) c) self-similar solutions to the equations.

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MS10

Microbial-Induced Mineralization in Biofilms

One of the salient features of biofilms is their spatial heterogeneity; they are not uniform, well-mixed systems like many laboratory microbial communities are. Because of spatial variation, advective and diffusive processes become influential. Further, when ionic quantities are important, these processes in turn can lead to electric field effects becoming significant. These issues are discussed in the context of a particular phenomenon, namely mineralization resulting from biological activity in biofilms. We present a multiphase model of this process.

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MS10

Reactor Scale Flow Effects and How They Affect Biofilm Activity

Bulk flow hydrodynamics is known to have primarily two effects on biofilm processes: 1) It applies mechanical shear forces to the biofilm and causes it to deform and eventually to detach, and 2) it contributes to convective transport of beneficial and harmful dissolved substrates to the biofilm and dissolved biofilm products from the biofilm. In laboratory experiments, bulk flow hydrodynamics depends largely on the biofilm reactor used for a study and on the operating conditions. Hence mesoscopic biofilm scale processes are critically influenced by macroscopic reactor scale conditions. In this talk we will give a brief overview of commonly used biofilm laboratory reactors and show, using numerical simulations, how reactor type and operating conditions can affect mass conversion and population dynamics in biofilms. This is joint work with Rangarajan Sudarsan (Guelph) and Gideon Wolfaardt (Ryerson).

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MS11

Diversity and Emergence Approaches to Cybersecurity

It is well understood that cyber security problems are exacerbated if not rooted in complexity. Indeed, analogies drawn from other complex systems, such as biology (e.g. viruses) are common. An approach based on complexity theory will be presented that yields statistics for quantifying improvements in security. Turing Completeness and Undecidability require that baseline probability of compromise for an arbitrary code cannot be assessed rigorously. These methods however can unambiguously quantify a statistical improvement in security.

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MS11

Mathematically-based Approaches to Building Secure Cyber Systems

It is now clear that the conventional simulate-and-test approach is inadequate to build truly secure cyber systems. A promising alternative is to specify a mathematical model of what the system is supposed to do, and with the help of computer proof tools formally verify once-and-for-all that the implementation meets its specification. I'll give a sampling of the state-of-the-art in this field and some current research challenges.

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MS11

Cyber Security Experimentation: Gory Detail or None at All

Unique facets confronted by current cyber security analysis efforts are: tremendous pace of change of ground rules (axioms), apparently wide and deep phenomenological effects, and widely-varying interpretations of security objectives. Together, effective methods for cyber security analysis appear to be swung between two extremes: experimentation-based methods with full, gory detail, and abstraction-based methods with significant simplifications. In the case of methods in between, accuracy considerations make intermediate methods tend to swing rapidly back towards full detail, while scientific inquiry and efficiency considerations tend to swing them back towards abstractions. Based on our experience and past evidence, we argue that experimentation with gory detail is the most effective approach in the short- to medium-term, while the other extreme is relevant one for the longer term. Feasibility will be shown of sustaining the scale and fidelity for the former extreme, namely, experiments with full gory detail.

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MS11

A Proposed Trusted Open Source Process

In this talk we introduce a new 'trusted source' process to identify malicious code. This process provides a framework for positive validation of a clean system by tracking the source author of all executable code, as opposed to negative validation, asserting a clean system by the absence of malicious code evidence. We present a simulated application of this process to demonstrate how a commodity laptop could be validated as a trusted source system, using entirely open source software (i.e. a trusted open source computing platform). The resulting trusted open source system consists of a boot environment (coreboot), bootloader (Linux boot kernel), virtual machine hypervisor (Linux+kvm), Linux kernel, and a user environment in which every byte of executable code can be traced back to trusted, multi-source verifiable, and cryptographically signed source code. This environment enables a complete positive validation of the system, ensuring the absence of malicious code. In general, this process can also be applied to proprietary sources, or other code which can not be publicly disclosed. We have chosen open source as a starting point because of ease of access to data about software developer social networks and open historical records of software development in multiple redundant repositories and mailing lists. We anticipate the use of advanced data mining techniques, social modeling, and other cutting edge techniques in the development of this framework.

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MS12

Parallel Adaptive Solution of Coupled Viscous Flow and Transport

Over the past several years, we have been developing the parallel adaptive framework libmesh to enable a broad class of parallel adaptive multiscale-multiphysics simulations. This open-source framework has also been integrated with the software library Dakota for related uncertainty quantification studies. The present work describes progress in modeling and simulation of large-scale coupled flow and transport processes such as those arising in high speed compressible gas dynamics. This problem class is of central interest to the studies initiated in 2008 by our new DoE Center for Predictive Engineering Computational Sciences (PECOS). Numerical studies with libmesh and Dakota will be presented to demonstrate the main ideas and capability for engineering applications. Finally, the CSE capability for fundamental science studies will be briefly illustrated for a second problem class corresponding to Rayleigh-Benard-Marangoni cellular behavior in coupled viscous flow and heat transfer with thermo-capillary surface tension effects. References: [1] B. Kirk, J.W. Peterson, R. Stogner, and G.F. Carey, libMesh: A C++ library for parallel adaptive mesh refinement/coarsening simulations, Engineering with Computers, Vol. 22, 237-254, 2006. [2] M.S. Eldred, B.M. Adams, D.M. Gay, and L.P. Swiler, DAKOTA: A multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification and sensitivity analysis, Sandia National Lab. Report, edition 4.1.

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MS12

A Posteriori Analysis of Multiscale Operator Decomposition

Multiscale operator decomposition (MOD) is perhaps the most widely used technique for obtaining accurate numerical solutions of multiscale, multiphysics problems. In MOD, a model is decomposed into components involving simpler physics over a limited range of scales, and a solution of the entire system is computed using numerical solutions of the individual components. MOD has many appealing aspects for problems with multiple scales and physical processes. However, MOD affects both accuracy and stability in both ways that are difficult to quantify accurately. In recent years, we have extended adjoint-based a posteriori analysis techniques to a variety of MOD methods. I will present a few examples that illustrate the possible effects from MOD and give a brief overview of the new developments in a posteriori error analysis.

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MS12

New Approaches to Codes and Computing Systems for Multi-PetaFLOP/s UQ Applications

ASC Sequoia scheduled for delivery to the Tri-Laboratory community in 1H2011 will provide a world class platform for Uncertainty Quantification (UQ) studies in support of the Stockpile Stewardship program. In this presentation, we discuss new approaches that ASC are taking to UQ and their impact on UQ Frameworks, applications, ASC Sequoia and future Exascale systems designs. Thinking about these three conjoined topics holistically for the next couple of generations of UQ applications provides the opportunity to address old problems in fundamentally new ways. In particular, we discuss new approaches to the problems of parallel programming, application resiliency and large scale data storage and analysis.

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MS12

C^1 Finite Element Analysis of Surfactant-Driven Thin Film Flow

As the thickness of a fluid film tends to zero, previously negligible effects begin to control the flow physics. For the thinnest fluid films, a dominant physical effect is surface tension. Surface tension is dependent on surface chemistry and temperature, and thin fluid film flow can be stabilized or driven to instability by the application of heating or the addition of surfactant. Depth-averaging the incompressible flow equations results in a two-dimensional, fourth-order nonlinear transient PDE describing the evolution of film thickness. The presence of surfactant leads to a second, coupled fourth-order equation describing dilute surfactant transport. This coupled multiphysics model is discretized and solved using a conforming C^1 finite element approximation on non-conforming adaptive grids. Analysis and results are presented.

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MS13

A Physics Based Approach to Radar Waveform Design

We show the relationship between radar waveform design and nonlinear filtering, with special emphasis on real time computational complexity. We focus on the design of optimal space-time waveforms for MIMO radars, considering the important physical constraint of radiation of at least 90% of the energy into real space, as well as good signal-to-clutter ratio, minimal loss in SNR, low range-Doppler sidelobes, robustness to uncertainty in Doppler, as well as low real time computational complexity.

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MS13

The Measurement Problem in Radar: What can we Observe from the Return Waveform?

Radar waveform design is typically based on the Woodward ambiguity functionwhich in turn is based upon the idealization that the effect of interaction on the transmitted waveform is a delay and a Doppler shift. With modern waveforms, it is possible to consider interactions from the perspective of operators which create functional changes on the radar waveform. We suggest new approaches to waveform design based on this observation.

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MS13

Generalized Huygen's Principle Using Pulsed Beam Wavelets

Huygens' principle is generalized so that any spatially bounded time-dependent source can be represented as a sum of pulsed beams radiated from a closed surface surrounding the source. The spherical "Huygens wavelets" are thus replaced with highly directed pulsed beams. This results in a highly compressed representation of radiation fields obtained by ignoring all beams missing a given observer. The compression ratios thus attainable with minimal error are quite stunning.

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MS13

Autocorrelation and Modulus Constraints in Radar Waveform Optimization

Abstract unavailable at time of publication.

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MS14

Design of Coated Stents in Interventional Cardiology

Stents are used in interventional cardiology to keep a diseased vessel open. New stents are coated with a medicinal agent to prevent early reclosure due to the proliferation of smooth muscle cells. This paper focusses on the asymptotic behavior of the dose for general families (normal tiling) of coated stents under a fixed ratio between the coated region of the stent and the targeted region of the vessel and set therapeutic bounds on the dose.

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MS14

Shape and Topology Optimization in Geometrical Inverse Problems and Imaging

In this talk an overview of the use of shape and topological sensitivity analysis in geometric inverse problems (such as electrical impedance tomography), image processing (such as segmentation and denoising) and optimal control and design problems (such as optimal design subject to variational inequalities) is provided. The use of these tools in level set based numerical realization is discussed and results are given.

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MS14

An Efficient Algorithm for Shape Optimization on Elliptic Eigenvalue Problems

We will present an efficient numerical approach to find the optimal shape and topology for elliptic eigenvalue problems in an inhomogeneous media. The method is based on Rayleigh quotient formulation of eigenvalue and a monotone iteration process to achieve the optimality. Due to the binary update, our method not only has the ability of topological changes but also is exempt from CFL condition. We provide numerous numerical examples to demonstrate the robustness and efficiency.

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MS14

Polygons as Solutions to Shape Optimization Problems with Convexity Constraint

In this work, we focus on the following general shape optimization problem:

$$\min\{J(\Omega),\ \Omega\ convex,\ \Omega \in \mathcal{S}_{\dashv\lceil}\},$$

where $\mathcal{S}_{\dashv\lceil}$ is a set of 2-dimensional admissible shapes and $J : \mathcal{S}_{\dashv\lceil} \to \mathbf{R}$ is a shape functional.

Using a specific parameterization of the set of convex domains, we derive extremality conditions (first and second order) for this kind of problem. We use these optimality conditions to prove that, for a large class of functionals (satisfying a concavity like property), any solution to this shape optimization problem is a polygon.

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MS15

On Wave Equations with Interior and Boundary Interactions between Supercritical Sources and Damping Terms

The model under consideration is the semilinear wave equation with supercritical nonlinear sources and dampings and our aim is to discuss the wellposedness of the system on finite energy space H1() L2(). A distinct feature of the equation is the presence of the double interaction of source and damping, both in the interior of the domain and on the boundary. Moreover, the nonlinear boundary sources are driven by Neumann boundary conditions. Since Lopatinski condition fails to hold for dimension of the domain greater or equal to two, the analysis of the nonlinearities supported on the boundary, within the framework of weak solutions, is a rather subtle issue and involves strong interaction between the source and the damping. I will provide positive answers to the questions of local existence and uniqueness of weak solutions and moreover give complete and sharp description of parameters corresponding to global existence and blow-up of solutions in finite time.

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MS15

A High Performance Computational Tool for Multiscale Multiphysics Simulation

Using the hydrodynamic code FronTier, we have developed a model to study through simulations, Type Ia supernova. Here we first present the algorithm and its effectiveness and efficiency. Then we present the results that we have obtained by using this algorithm to study a type Ia supernovae. The study is based on a sharp flame model that is free of adjustable turbulent transport parameters.

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MS15

Effects of Small-scale Fluid Motion on Planktonic Organisms: How Spines can Affect Fluid/cell Interaction

We study plankton with spines because spines have numerous fluid dynamic consequences, such as more surface area for pressure and shear stress to act over and increased volume of fluid that interacts with the cell. We apply a model based on the immersed boundary method to simulate and explain this complex plankton-fluid system. Different kinds of shear flows are imposed for comparison of real plankton behavior and motion predicted by fluid physics.

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MS15

Geometry of Cophylogeny

A cophylogeny is a pair of phylogenetic trees satisfying some given conditions. Cophylogeny theory allows us to study two trees with related structure, such as a gene tree and a species tree, without assuming their independence. In this talk, we introduce several spaces of cophylogenies. We also give some combinatorial results about possible cophylogenies, in the case where one tree of the cophylogeny is a host tree and the other is a parasite tree.

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MS16

The Electromagnetic Field Generated by a Moving Plasma and the Feynman-Lienard-Wiechert Formulas for a Moving Point Charge

The speaker establishes formulas for the electomagnetic potential and current associated with a plasma flow, based on a time delay function that represents the plasma's arrival at the past light cone. These formulas generalize and include formulas of Feynman and Lienard-Wiechert to be found in Volume 2 of the Feynman Lectures in Physics.

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MS16

Pre-metric Electromagnetism and Emergent Gravity

At present it is customary to regard the geometry of the spacetime manifold as defined by the Lorentzian metric tensor field that accounts for the presence of gravitation. In the pre-metric formulation of electromagnetism the fundamental objects are the spacetime volume element and the electromagnetic constitutive law. The Lorentzian structure appears as a degenerate special case of the dispersion law for electromagnetic wave propagation that follows from the pre-metric Maxwell equations. Hence, gravity represents a consequence of the more fundamental electromagnetic structure of spacetime.

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MS16

Distribution Theory Applied to the Electromagnetic Field due to a Charged Particle

Abstract unavailable at time of publication.

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MS16

Absence of a Consistent Classical Equation of Motion for a Mass-renormalized Point Charge

The restrictions of analyticity, relativistic rigidity, and negligible $O(a)$ terms are taken into account to obtain a classical equation of motion of an extended charge that is both causal and conserves momentum-energy. However, renormalization of the electrostatic mass to a finite value as the radius a of the charge approaches zero introduces a violation of momentum-energy conservation into the equation of motion of the point charge if the magnitude of the external force becomes too large. That is, the causal classical equation of motion of a point charge with renormalized mass experiences a high acceleration catastrophe.

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MS17

The Population Dynamics of Coupled Neurons in a Finite-size Network

Coupled neurons are usually studied in either the context of small networks or in the limit of infinitely large mean field networks. However, the interesting and biologically relevant regime of large but not infinite networks has not been as well explored. Here I will present some different approaches and results for the dynamics of finite-size neural networks.

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MS17

A Diagrammatic Expansion of Pulse-coupled Network Dynamics in Terms of Subnetworks

I will introduce a framework wherein various long-time measurements of a pulse-coupled network's stationary dynamics can be expanded in terms of that network's connectivity. Such measurements include the occurrence rate of pulses as well as higher order correlations in activity between various neurons in the network. The various terms in this expansion can be interpreted as diagrams corresponding to subnetworks of the original network which span both space (in terms of the network's graph) as well as time (in the sense of causality).

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MS17

Multi-phase Rhythms in Neuronal Networks with Multiple Timescales

There are a variety of mechanisms through which simple neuronal networks can produce similar activity patterns. Here we discuss ways in which different intrinsic characteristics within networks exhibiting similar multi-phase dynamics, involving multiple timescales, yield different phase-switching mechanisms and responses to variations in inputs. Our results combine singular limit analysis and numerical identification of bifurcations in systems with several slow variables.

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MS17

An Exploration of Bursting Mechanisms in Olfactory Bulb External Tufted Cells

Recent experiments by Liu and Shipley (J. Neuroscience 2008) identify several intrinsic currents involved in bursting activity in synaptically isolated external tufted (ET) cells of the olfactory bulb. Here we present a multi-compartment model of endogenously bursting ET cells. We explore possible mechanisms underlying different burst patterns, with a particular focus on potential modulatory targets responsible for the wide range of interburst intervals observed empirically. Our methods include automated parameter estimation techniques which utilize geometric features underlying bursting.

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MS18

Large-scale Simulation in Petascale Computing

This talk will cover our experience over the last several years at TACC operating and using Ranger, one of the largest supercomputers in the open science community. Aspects of performance, optimization, and profiling on these large-scale cluster architectures will be described. A variety of application performance results from a wide range of computational science communities will be presented. Also discussed will be a number of lessons learned during the deployment, operation, and support of these systems.

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MS18

Multilevel Parallelism in Unstructured Adaptive Finite Element Algorithms

The landscape of supercomputing has changed over the past decade with the transition from purpose-built machines with custom processors to today's massively parallel machines using commodity chips. Today's commodity multicore chips, however, present a significant departure from the traditional processor architecture. This presentation will discuss the issues driving the trend to multicore, the implications for scientific computing, and approaches for addressing the multilevel parallelism available in today's machines. As a case study, the multilevel parallelism which is being implemented in the libMesh finite element library will be discussed.

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MS18

Modeling of Reactive Wetting and Spreading

Wetting, phase change and reaction in high temperature systems (e.g., a liquid metal on a metal substrate) are complex phenomena that are only partially understood. These phenomena are key to joining processes, thin film processing and sintering among others. Reactive wetting is characterized by chemical and physical processes that span a broad range of spatial and temporal scales. Models of reactive wetting incorporate knowledge from chemical thermodynamics, phase transformations, capillary behavior and multi-phase transport. A framework of sequential multiscale models provides a necessary foundation for the future development of more fully-coupled multi-scale models. At present, the modeling consists of an advection- diffusion model at the drop scale, a diffuse interface model coupled to hydrodynamic transport at the macro- and meso-scopic scales and molecular dynamics modeling of wetting and dissolution of high temperature metal-metal systems. The models are used to simulate wetting and dissolution of a spreading liquid metal drop on a metal substrate. Simulation results for the extent of spreading are compared to experimental observations.

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MS18

A Parallel Finite Element Model for Hurricane Storm Surges

Recent hurricane events in the Gulf of Mexico have demonstrated the vulnerability of coastal populations and infrastructure to storm surges. A high fidelity storm surge model includes an accurate definition of the physical system, incorporation of all relevant physical processes, numerical resolution of all pertinent flow scales and robust and accurate solution of the resulting system of PDE. We discuss the ADCIRC finite element model, outline the computational methodology to approximate the solution, and give numerical results.

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MS19

Efficient One-Shot Methods for Aerodynamic Shape Design

Different one-shot optimization methods for aerodynamic shape design problems will be presented. These methods enable aerodynamic shape designs for the computational effort of a small, constant multiple of the effort of an aerodynamic simulation. Integral part of these approaches are gradient preconditioning and shape derivatives.

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MS19

Second-order Topological Expansion for Electrical Impedance Tomography

Second-order topological expansions in electrical impedance tomography with piecewise constant conductivities coefficients are considered. First order expansions usually consist of local terms involving the state and the adjoint solutions and their gradients. In the case of second-order topological expansions, non-local terms appear. Interactions between several simultaneous perturbations are also considered. The study is aimed at determining the relevance of these non-local and interaction terms from a numerical point of view.

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MS19

Topological Sensitivity Analysis Applied to the Topology Design of Microstructures

This paper deals with the sensitivity analysis of the macroscopic elasticity tensor to topological microstructural changes of the underlying material. The derivation of the proposed sensitivity relies on the concept of topological derivative, applied within a variational multi-scale constitutive framework. The obtained derivative is used to devise a class of topology optimization algorithm which is applied to the synthesis and optimal design of microstructures to meet a specified macroscopic behavior.

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MS19

Efficient Aerodynamic Design by Use of the Shape Calculus

Optimal aerodynamic design is most often treated by parametric approaches. Besides geometric inflexibility, one is also faced with loss of efficiency due to practically unavoidable mesh sensitivities. The shape calculus enables to circumvent both problems and leads to highly efficient numerical methods, if characteristic parts of the shape Hessian are used in addition to the shape gradient. Results for industrially relevant test cases are presented.

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MS20

Computing Statistical Averages via Dynamical Zeta Functions and Hyperbolic Periodic Orbits

Abstract not available at time of publication. We present the use of hyperbolic periodic orbits and dynamical zeta functions in computing time averages for observables in ergodic attractors supporting hyperbolic measures. We present concrete results for the Lorenz attractor, and discuss some theoretical and computational hurdles in applying the approach to attractors in higher dimensional spaces.

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MS20

Stochastic Nonlinear Models of Interpersonal and Romantic Relationships and Strange Attractions

More than 50% of the United States adolescents have been in some form of romantic relationships. Current theories from biosocial, ecological, and interpersonal frameworks are grounding romantic relationships in normative social experiences. However, these theories have not been developed to the point of providing a solid theoretical understanding of the dynamics present in relationships, and integrative theories are still lacking. We present mathematical models (both deterministic and stochastic) to examine behavioral features associated with relationships.

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MS20

Fused SVM Classification of Temporal Gene Expression Responses to Endotoxin

The human endotoxemia model is a powerful tool to analyze in vivo biological responses that unfold during the acute phase of systemic inflammation. Using Support Vector Machines(SVM), we learn a model that predicts the state of endotoxin exposure in a patient using gene expression profiles. Fused-SVM penalizes complex models via a regularizer that assigns similar weights to temporally adjacent expression values. We identify genes that are strong predictors for the acute phase of systemic inflammation.

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MS20

Soliton Solutions of the Kadomtsev-Petviashvili Equation

This research project involves the study of a weakly two dimensional version of the Kortweg-deVries equation, known as the Kadomtsev–Petviashvili (KP) equation. The KP equation models nonlinear wave interactions in shallow water which can cause extremely high elevation waves on the ocean surface. There exist many different classes of solutions for the KP equation, however the focus of this research work is on the so called line-soliton solutions. Along with the structure of two specific 2-soliton solutions, the relationship between the angle of interaction and amplitude is presented.

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MS20

Analysis of Asymmetric Stable Droplets in a Fish Patterning Model

Soliton like structures called "stable droplets" are found to exist within a paradigm reaction-diffusion model which can be used to describe the patterning in a number of fish species. It is straightforward to analyse this phenomenon in the case when two non-zero stable steady states are symmetric, however the asymmetric case is more challenging. We use a recently developed perturbation technique (Gomila et al, 2004 D. Gomila, P. Colet, G. L. Oppo, and M. S. Miguel. Stable droplets and nucleation in asymmetric bistable nonlinear optical systems. J. Opt. B: Qauntum Semiclass. Opt. 6, 6(5):265-270, 2004) to investigate the weakly asymmetric case.

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MS20

-Centered Poisson Solvers and Multilevel Summation Algorithms

We consider the problem of efficiently calculating the electrostatic field of a molecule immersed solvent, as described by an implicit solvent model based on the Generalized Poisson Equation (GPE). An equivalent integral equation formulation for GPE is derived, in order to reduce domain of interest to the molecular boundary. The integral equation is discretized using a projection method, and the resulting linear system is solved using BiCGStab. Each step of BiCGStab requires the evaluation of a discrete integral transform with a non-local kernel, which has quadratic computational complexity when handled by a naive algorithm. However, this can be reduced to linear complexity using the Multilevel Summation Method (a fast N-body solver). We show both numerically and theoretically that the resulting GPE solver scales linearly for a given accuracy level.

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MS21

An Abstract Model for Programming Multi-core Nodes

We outline an abstract node API to support the implementation of large-scale linear algebra primitives on a wide-range of HPC architectures. This API is primarily concerned with the issues related to memory management, data communication, and computational abstraction that arise in support of architectures employing a mixture of distributed, SMP/multi-core, and attached processors (GPU/Cell). This discussion takes place in the context of Tpetra, a templated next-generation implementation of the Epetra parallel linear algebra library in the Trilinos project.

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MS21

Programming on the Path to Peta-scale

As computers scale up to hundreds of thousands of cores, develop deeper computational and memory hierarchies, and increased heterogeneity, developers of scientific software are increasingly challenged to express complex parallel simulations effectively and efficiently. In this talk we will examine a broad set of applications running on the peta-scale Cray XT at Oak Ridge National Laboratory. Performance data will be presented illustrative of their history of computation leading up to simulations running on over 100,000 processor cores. We will examine their performance trends over this time, as well as the ways in which the codes developed as a means of attaining this scale of computation. We will discuss how they might evolve in order to take better advantage of the scale and complexity of these architectures. This includes a discussion of the developing capabilities of the MPI-3 specification, our experiences using the developing HPCS languages as well as other alternatives, such as UPC, shmem, Co-Array Fortran, and OpenMP.

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MS21

Parallel Multiscale and Multiresolution Computations in Computational Chemisty and Nuclear Physics

We describe MADNESS, a parallel and scalable dynamic adaptive pseudo-spectral multiresolution environment for solving nonlinear Schrodinger equations and density functional theory in computational chemistry and nuclear physics in three and higher dimensions. One of the key features is an unique adaptive representation for each of the wavefunctions. To overcome the overwhelming complexity of programming parallel computers, MADNESS software employs a parallel runtime architecture which removes from the programmer the responsibilities of managing dependencies, placement of data, and scheduling of computation. This hides from the programmer much of the machine complexity and enable them to concentrate upon the high-level algorithms and expressing concurrency. The runtime efficiently overlaps computation and communication and targets multicore and future hybrid devices.

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MS21

Scalable Computing Challenges: An Overview

Petascale systems and their successors pose unique challenges for algorithm and application developers. The introduction of multicore–and soon manycore–nodes add a new dimension of scaling that must be addressed new ways. Furthermore, these systems will have many nodes, which will challenge effective use by a single application. Finally, system reliability will likely degrade, requiring more sophisticated resilience techniques than simple checkpoint-restart. This overview presentation will highlight the particular challenges that these systems pose for algorithm research and development. We will also discuss software design changes that can be effective in preparation for manycore architectures.

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MS22

An Optimization Approach for Fitting Canonical Tensor Decompositions

Tensor decompositions are higher-order analogues of matrix decompositions and have proven to be powerful tools for data analysis. In particular, we are interested in CANDECOMP/PARAFAC (CP) model, which expresses a tensor as the sum of rank-one tensors. The problem of computing the CP decomposition is typically solved using an alternating least squares (ALS) approach. Previously, nonlinear least squares (NLS) methods have also been recommended. We discuss the use of gradient-based optimization algorithms for fitting the CP model and demonstrate that these are more accurate than ALS and faster than NLS.

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MS22

Performance Optimization Issues in the Automatic Synthesis of High-Performance Codes for Tensor Contraction Expressions in Quantum Chemistry

The Tensor Contraction Engine (TCE) is a compiler that translates tensor contraction formulas for a class of quantum chemistry computations into Fortran code delivering high levels of performance tailored to the characteristics of the target architecture. We give an overview of the architecture of the TCE and describe the optimizations performed by the TCE and its runtime libraries.

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MS22

Applications of Tensor Decompositions in Chemometrics

Tensor decompositions have been used in chemometrics for the past 30 years. Applications include the PARAFAC model (low-rank approximation of an arbitrary N-way tensor), Tucker models (a derivation of higher-order SVD) and several models with intermediate properties. Some examples with the state-of-the-art algorithms and applications of tensor models in chemistry will be presented.

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MS22

A Jacobi/Sweep Algorithm for Certain Very Large Quantum Chemistry Eigenproblems

A Jacobi-Davidson type method is presented for computing the smallest eigenvalue and associated eigenvector of a very large Hamiltonian that is a highly structured summation of Kronecker products. The vector iterates are represented in compressed form using tensor networks. Updates involve a succession of orthogonal matrix manipulations and projections.

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MS23

Modeling Integrin Activation in Initial Cell Movement

Cell motility is an essential process in the life cycle of many organisms, as it plays a crucial role in a variety of areas such as embryonic development, wound healing, the immune response, and cancer cell metastasis. Furthermore, errors during cell migration have serious consequences including mental retardation, vascular disease, tumor formation, and metastasis. Therefore, an understanding of the mechanism by which cells migrate may lead to the development of novel therapeutic strategies for controlling, for example, invasive tumor cells. Cells adhere to and move across their surroundings via protein complexes known as focal adhesions (FAs). FAs serve both as mechanical links from the cell to its surroundings (via transmembrane integrin receptors) and as biochemical signaling hubs to concentrate and direct numerous signaling proteins within the cell. Here we present a mathematical model to describe the early dynamics of these focal adhesions in mammalian cells to determine the necessary components and the role of each (with a particular emphasis on the activation of integrin receptors) in the growth and fate of the FAs.

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MS23

Multistable Dynamics Mediated by Tubuloglomerular Feedback in a Model of a Compliant Thick Ascending Limb

In single nephron filtration, micropuncture studies demonstrated the existence of oscillatory states mediated by tubuloglomerular feedback. We study these oscillations whose role is to regulate fluid delivery into renal tubules. Bifurcation analysis revealed different parameter regimes where the flow perturbations can elicit stable oscillations with various frequencies: f, 2f and regimes with mixed frequencies of I and 2f.

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MS23

HER2 Effects on Cell Behavior: A Mathematical Model

To investigate the effects of HER2 receptor overexpression on cell proliferation, we have developed a mathematical model that describes the proliferative behavior of HER2-overexpressing cells as a function of the HER2 level. The proliferation model formulates the cell proliferation rate as a function of the cell surface HER2 and EGFR levels. Numerical simulations of the model give good agreement with the experimental data in which an increase in HER2 receptors leads to increased cell proliferation.

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MS23

The Role of Substrate Rigidity on Pattern Formation of Endothelial Cells Movement in Tumorinduced Angiogenesis

In recent years, tumor induced angiogenesis has become an important field of research representing a crucial step in the development of malignant tumors. A better understanding of its steps may contribute to the development of new cancer therapeutic strategies. We present a hybrid model for the capillary tube formation of endothelial cells treated as discrete units in a continuum field of a chemoattractant and the effect of the substrate rigidity in the final networks topology.

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MS24

Are Standardized Test Scores Biased Against Minorities?

College admissions offices across the country use standardized test scores to allocate educational opportunity. Critics argue that test scores are biased against minorities, which from a statistical perspective suggests that tests scores differentially predict college performance. This study develops a model for approximating the probability that researchers and/or practitioners would identify unfairness against minorities. The developed model shows that various design artifacts interact to decrease the chances that commonly employed statistical methods will detect unfairness.

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MS24

Non-negative Matrix Factorization: The Extreme Data Property and Ill-Posedness

Identifying the components of a dataset is a fundamental problem in science and engineering. Non-negative Matrix Factorization (NMF) is a mathematical tool for performing this complicated task. Unfortunately, the non-negativity constraints prevent many well-developed linear algebra algorithms, such as the singular value decomposition, from being applicable to NMF. In this talk, an alternative algorithm for performing NMF is developed using the geometry of the problem and raising questions about the ill-posedness of the NMF problem.

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MS24

A Multistate Asynchronous Model of the Canonical Wnt Pathway

The canonical Wnt Pathway consists of cell-surface receptors that bind to Wnt proteins and ultimately lead to a change in the amount of beta-catenin in the nucleus which in turn regulates several cell functions. We describe a multistate asynchronous model of the interaction network comprised of proteins utilized in the Wnt pathway, cell proliferation, apoptosis, and differentiation. This model is then used to detect signaling abnormalities in the interaction network due to mutations in APC.

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MS24

A Stochastic Model of Gene Regulation

We consider a simple gene regulatory network consisting of one gene and a set of proteins that regulate its expression. When the number of regulatory proteins in the system is large, a Hill function is typically used to model regulation of gene expression, but this breaks down for low numbers of protein due to stochastic effects. We investigate the type of function that should be used in place of the Hill function.

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MS25

Some Challenges on High Resolution Climate Simulations

We work with a state-of-the-art atmospheric general circulation model and here we present some of its computational challenges. We look at the objectives in climate modeling and some of the proposed numerical solutions, and compare different discretization schemes and solvers.

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MS25

Solving Ab-initio Nuclear Structure Problems with Configuration Interaction Methods

We perform ab-initio no-core calculations for nuclear structure using basis function expansion methods on massive parallel computers. The nuclear many-body Hamiltonian can be expressed as a large, sparse, symmetric matrix, which we solve for the lowest eigenvalues and eigenvectors; we have obtained the ten lowest eigenvalues of matrices of dimension two billion. The eigenvalues give us the binding energy of the system; the eigenvectors are used to calculate additional experimental quantities.

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MS25

Enabling Robust and High-fidelity Accelerator Modeling using Advanced Computing

Accelerators are crucial in many areas of research. Existing and proposed accelerators, such as Compact Linear Collider, Linac Coherent Light Source, and Facility for Rare Isotope Beams, have components with complex geometries. High fidelity and robust modeling and simulation are needed not only to reduce the cost of the design and construction, but also to ensure safe and efficient operation of such accelerators. In this talk, we will give an overview of the challenges of accelerator modeling and describe the role of advanced computing in the simulation.

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MS25

Linear Scaling Electronic Structure Calculations for Tens of Thousands of Atoms Using Hundreds of Thousands of Processors

A linear scaling three dimensional fragment method for electronic structure calculation will be presented. This method divides a system into small fragments, calculates the energies and the charge densities of the fragments independently, then patches them together with a novel scheme which cancels out the artificial surface effects. The method scales to hundreds of thousands of processors, and can be thousand times faster than a direct density functional theory calculation with essential the same results.

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MS26

Optimal Response to Cyber Security Attacks

Cyber Security is a growing concern especially in open grids, where attack propagation is easy due to existing collaborations. We consider how to optimally respond to an attack in grid environments. We present an optimization model that takes the existing collaborations as input and that minimizes the disruption to the grid whilst reducing threat-levels at unaffected sites. Our optimization model outputs which collaborations must be suspended or monitored to reduce threat-levels at sites and overall.

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MS26

Anomaly Detection in Computer Network Traffic Using Graph Based Scan Statistics

We propose a framework for anomaly detection in computer network data. The model is a bursty Poisson process model. The bursts in rate are parameterized by a two state Markov process. Maximum likelihood estimates for the birth and death parameters and baseline rates are obtained. Finally, anomaly detection is accomplished using scan statistics across time and the graph derived from the network. Anomalous clusters of events can be detected in this way.

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MS26

The Mathematics Behind the Analysis of Software (Source code and Binaries)

The development of technologies for the analysis of software (both source code and binary executables) has combined both Computer Science (compilers) and Mathematics (equation solving) and come to depend heavily on both. The automation of the analysis of software is a critical step in addressing the scale of the demands to knowledge about the growing volume of software available. The acknowledgment that there is source code for some software but frequently not much of it, requires a broader approach within the analysis. The formulation of large scale sets of equations from aspects of the analysis of software serves to help understand the software and formulate equations to characterize its behavior. The support for the mathematics behind solving such systems of logic equations can be computationally intensive.

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MS26

A Chaos-mathematical Approach to Insider Threat Detection

We discuss our research on applied chaos mathematics for insider threat detection. We model the insider adversary's computer account as a nonlinear dynamic system, and subsequently apply techniques from chaos mathematics to find the underlying order of adversarial behavior, condition variables that largely characterize adversarial behavior, and input variables in a computing environment that affect adversarial behavior. We leverage such knowledge into adversarial behavior estimation and control algorithms, which we employ to probe insiders minds.

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MS27

Applying Global Constraints to Local Map Reductions of ODE Dynamics in a Spiking Biophysical Neural Network Model

Searching for parameter values and initial conditions that lead to desirable emergent behaviors in high-dimensional dynamical systems is like asking which arrangements of individual letters create a good novel: it's a question posed at the wrong scale. The appropriate objects underlying complex function are simpler dynamic motifs that are inherently qualitative in nature. We derive quantitative representations of such motifs for a classic biophysical neural network and analyze the logical interactions between them. This generates locally reduced maps coupled by global constraints, thus elucidating low-dimensional mechanisms at work in the system.

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MS27

Correlation Transfer in Neuronal Populations

Correlated activity in neural tissue can impact the information carried by neural populations. However, there are few results that provide a mechanistic understanding of their generation and propagation. We examine this question using versions of the integrate and fire model, extending previous results for single neurons to populations. We also present new numerical methods for the simulation of networks of stochastic integrate and fire neurons which are orders of magnitude faster than Monte Carlo simulations.

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MS27

Spike Train Statistics and Dynamics with Synaptic Input from Any Renewal Process: A Population Density Approach

In neural network modeling, a common assumption is that the arrival times of synaptic input events are governed by a Poisson process. This ignores temporal correlations in the input that sometimes have important physiological consequences. We formally and properly extend probability density methods of integrate-and-fire neurons to include synaptic input event times governed by any modulated renewal process. We study how the regularity of input spike train effects the statistics of the output spike train.

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MS27

Analyzing Neuronal Networks using Discrete Time Dynamics

We describe mathematical techniques for analyzing detailed biophysical models for excitatory-inhibitory neuronal networks. While these networks arise in numerous applications, the focus of this talk will be to better understand mechanisms that underlie temporally dynamic responses in the olfactory system. Our strategy is to first reduce the model to a discrete-time dynamical system. Using the discrete model, we can systematically study how the emergent firing patterns depend on parameters including the underlying network architecture.

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MS28

A Model for Single Phase Flow in Horizontally Fractured Porous Media using Homogenization Techniques

A double porosity model for single-phase flow is derived in a reservoir with horizontal fractures. The microscopic model consists of Darcy flow equations in the fractures and matrix. The matrix permeability coefficients are scaled according to the single, vertical direction of homogenization, preserving the physics of the flow between matrix and fracture as the matrix blocks shrink. Extracting weak limits of the microscopic model solution shows convergence to the macroscopic model.

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MS28

Multiscale Modeling for Seismic Inversion

Imaging the Earth's subsurface requires determination of the "important information' inherent in data that ranges over multiple scales. While numerical upscaling is a common approach for flow simulation, simulation of waves through the same Earth is generally accomplished using single scale finite differences. We describe a two-scale finite-element based wave simulator and the associated adjoint problem. This adjoint calculation is straight-forward if differentiation of the continuous pde model is accomplished before discretization using upscaling.

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MS28

The Narrow Fracture Approximation for Channeled Flow

The singular problem consisting of non-stationary Darcy flow in a region containing a narrow channel of width $\mathcal{O}(\epsilon)$ and high permeability $O(\frac{1}{\epsilon})$ is shown to be well-approximated by a problem with flow concentrated on a weighted Sobolev space over a lower-dimensional interface. The convergence of the solution as $\epsilon \to 0$ is proved. The structure of the limiting initial-boundary-value problem is dependent on the rate of taper of the channel.

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MS28

Multiscale Methods for Highly Oscillatory ODE

Abstract unavailable at time of publication.

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MS29

A Stochastic Newton Method for Statistical Inverse Problems Governed by PDEs

We present a Markov-chain Monte Carlo (MCMC) method for sampling high-dimensional, expensive-to-evaluate probability density functions that arise in the Bayesian solution of statistical inverse problems. The method builds on previous work in Langevin dynamics, which uses gradient information to guide the sampling in useful directions, improving acceptance probabilities and convergence rates. We extend the Langevin idea to exploit local Hessian information, leading to what is effectively a stochastic version of Newton's method. A large-scale inexact-Newton-CG variant is developed, analogous to methods used in PDE-constrained optimization. We apply the method to the Bayesian solution of an inverse problem governed by seismic wave propagation, for which we observe several orders of magnitude faster convergence over state-of-the-art blackbox MCMC methods.

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MS29

Problems of Design in Inverse and Control Prob-

lems

Abstract unavailable at time of publication.

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MS29

Preconditioners for All-at-once PDE-constrained Optimization

Saddle-point systems arise from most optimization problems with constraints. In this talk we will describe how such problems arise from optimization with constraints which are themselves discretizations of partial differential equations. Such problems are necessarily of very large dimension and matrix factorizations of any type must be avoided. We will describe optimal preconditioning strategies for such problems and show numerical results on certain test problems.

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MS29

Incorporating Bound Constraints into Monolithic Solvers for PDE Control

Optimal control problems with PDE constraints pose a serious computational task. The introduction of bound constraints for the control poses new methodological and numerical challenges. We present an active set and a projected gradient approach and discuss the arising linear systems in saddle point form. We present efficient preconditioning strategies and numerical results are shown.

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MS30

Winners To Be Announced

Abstract not available at time of publication.

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MS31

Advances in the Analysis of Asymmetric Data using DEDICOM

DEDICOM (decomposition into directional components) is an algebraic model that was developed in the psychometrics community with similarities to multidimensional scaling for the analysis of asymmetric arrays. Three-way DEDICOM contains extensions for the analysis of 3-way arrays or tensors. This presentation shows several algorithmic advancements for fitting DEDICOM to large 2-way and 3-way data sets and also shows illustrative examples of analyzing large directed graphs with or without edge labels (semantic graphs).

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MS31

Nonlinear Approximations by Exponentials in Multiple Dimensions

We explore algorithms for nonlinear approximation of functions of several variables or multidimensional data by exponentials. In doing so, we extend our previous, one-dimensional results on nonlinear inversion of bandlimited Fourier transform of functions or data, where such approximations lead to efficient representations.

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MS31

Block Term Decompositions: Definition, Computation and Applications

Block Term Decompositions unify the two most well-known types of tensor decomposition, namely the Parallel Factor / Canonical Decomposition and the Tucker Decomposition. We discuss the computation by (i) alternating least squares optimization, (ii) exact line search, and (iii) Levenberg-Marquardt optimization. We mainly focus on applications in wireless communication. Time permitting, we discuss a scheme for the determination of the block dimensions.

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MS31

Diagrammatic Reduction of SU(N) Tensors with 'Birdtracks'

Group theory and tensors have become fundamental concepts in quantum physics. The reduction of tensors into their irreducible components is therefore an important ingredient for many calculations in this field. 'Birdtracks' are a Feynman diagram inspired notation for tensor calculus that avoids the usual proliferation of indices associated with traditional tensor calculus. We use these diagrams to implement an algorithm for the reduction of SU(N) tensors.

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MS32

Coarse Scale Adjoint Methods for Time Dependant Multiscale Problems

Adaptive error control for time dependent problems, especially problems with multiscale aspects, is a challenging problem, both from a standpoint of analysis and the computational implementation. We present an error control framework based on coarse scale adjoints that is used to guide and reduce fine scale residuals. Positive and negative examples of the framework are given. Modifying the framework leads to a variety of different multiscale approaches. We hypothesize on the class of problems where this multiscale algorithm works well and connect this broad framework with earlier work on block adaptivity and compensated domain decomposition for time dependent problems.

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MS32

Integrating Error Estimation, Adaptivity and Optimization

Algorithms for error estimation and adaptivity have been proposed in recent years using the PDE residuals weighted by the adjoint solution. At the same time, the adjoint approach has been used extensively in sensitivity analysis and optimization. We present recent work on algorithms for performing optimization under adaptive error control with emphasis on transient, multiphysics applications.

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MS32

An A Aposteriori Analysis of Operator Decomposition for Multiscale ODEs

We analyze an operator decomposition time integration method for systems of ordinary differential equations that present significantly different scales within the components of the model. With this formulation we derive both an a priori error analysis and a hybrid a priori-a posteriori error analysis. The hybrid analysis has the form of a computable a posteriori leading order expression and a provably-higher order a priori expression. Both analyses distinguish the effects of the discretization of each component from the effects of operator decomposition. The effects on stability arising from the decomposition are reflected in perturbations to certain associated adjoint operators.

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MS32

A Posteriori Error Analysis for Coupling Strategies of the Core and Edge Regions in the Tokamak Machine

We consider the a posteriori error analysis for multiscale domain decomposition problems where model systems of the equations in the core and the edge region in the tokamak machine are coupled through an interface. The equations in both regions are discretized by finite differences in time and finite volumes in space hence are reformulated in finite elements setting in both time and space in order to make use the variational framework for the a posteriori analysis. Various coupling strategies are discussed and analyzed.

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MS33

Fault Tolerance in Protein Interaction Networks: Stable Bipartite Subgraphs and Redundant Pathways

As increasing amounts of high-throughput data for the yeast interactome becomes available, more system-wide properties are uncovered. One interesting question concerns the fault tolerance of protein interaction networks: whether there exist alternative pathways that can perform some required function if a gene essential to the main mechanism is defective, absent or suppressed. One signature pattern for redundant pathways is the BPM (between-pathway model) motif, first suggested by Kelley and Ideker. Past methods proposed to search for BPM motifs have had several important limitations. First, they have been driven heuristically by local greedy searches, which can lead to the inclusion of extra genes that may not belong in the motif; second, they have been validated solely by functional coherence of the putative pathways using GO enrichment, making it difficult to evaluate putative BPMs in the absence of already known biological annotation. We show how a simple "folk" theorem in graph theory (probably due to Erdos) can help us identify possible BPMs in such a way that not only do we get better coherence of biological function, but we also have a direct way to validate our results based directly on the structure of the network. We uncover some interesting biological examples of previously unknown putative redundant pathways in such areas as vesicle-mediated transport and DNA repair.

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MS33

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MS33

In Search of Overlooked Functions: Hidden Connections Among Short Proteins

Most animal toxins are short proteins that appear in venom and vary in sequence, structure and function. Considering the appearance of homologous venom proteins in evolutionary remote species, it is plausible that homologues of such proteins may be found in non-venomous species as long as they fulfill some biological function. Indeed, sporadic instances of endogenous toxin-like proteins that function in non-venom context have been reported. Herein we show that many families of toxin-like proteins remain undiscovered. For the goal of discovering overlooked short functional proteins, we turned to developing a computational method that can characterize and thus detect such proteins. We have successfully utilized machine learning methodology, based on sequence-derived features and guided by the notion of structural stability, a common characteristic of toxins, in order to create a robust characterization of toxin and toxin-like proteins. We screen and applied large-scale search for these proteins in insect, mammalian but also less studied genomes. Our method detected dozens of putative novel toxin-like proteins. We will demonstrate a biological validation for some of these proteins. Furthermore, we show that the construction of a tree family scaffold of all proteins exposes hidden connections among many proteins many of them belong to viruses. We suggest that a systematically detection of viral protein families as well as toxin-like proteins may lead to novel pharmaceutical targets and to a deeper understanding of the evolutionary link between toxins, viral proteins and cell modulators.

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MS33

Balanced Minimum Evolution

I will explain the statistical motivation behind the balanced minimum evolution criterion in distance-based phylogenetics and review recent progress on understanding a greedy algorithm (the neighbor joining algorithm) for the criterion. This is joint work with Radu Mihaescu.

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MS34

Using Mathematical Models of Circadian Phase to Take the Lag out of Jet lag

Traveling across multiple time zones results in a decrease in human performance due to a desynchronization of the circadian system from environmental cues, the most important of which is light. We present an algorithm for designing light interventions with a limit-cycle model of circadian phase for jet-lag schedules that results in optimal predicted performance. The algorithm is shown to be optimal and results in theoretical predictions about the effect of shifting schedules on human performance.

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MS34

Periodic Forcing of a System Near Hopf Bifurcation

Forcing a system of ODEs near a point of Hopf Bifurcation by a per iodic signal whose frequency is near the Hopf frequency occurs in feed-forward networks and in models of the auditory system. We discuss aspects of the resonant responses in both cases.

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MS34

Multi-scale Analysis of Collective Decision-making in Informed Swarms: An advection-diffusion Equation with Memory Approach

We propose a multi-scale method for the continuum-level analysis of discrete, agent-based models of collective-decision making in swarms comprising a mixture of naive and informed individuals. The method is based on projecting the particle configuration onto a single meta-particle. The collective states of the configuration can be associated with the stochastic properties of the random walk of the meta-particle. The transport properties of the meta-particle can be correctly predicted with an Advection-Diffusion Equation with Memory.

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MS34

A Hodgkin-Huxley-type Model Orexin Neuron

Narcolepsy is associated with signaling loss in the orexin system. We developed a Hodgkin-Huxley-type mathematical model of the orexin neuron and modeled the seven experimentally-identified intrinsic currents. To explore local synaptic effects, we simulated small networks of orexin neurons with colocalized orexin/dynorphin coupling. The model properties are consistent with reported orexin electrophysiology including a depolarized resting membrane potential and spontaneous spiking (3-4 Hz). Small network analysis suggests time dynamics of dynorphin desensitization determine network behavior.

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MS35

Models of the Human Tear Film During the Blink Cycle

Lubrication models for the tear film are discussed in one and two spatial dimensions. In 1D, blink cycle results are presented; notions of a full blink and periodic solutions are linked. In 2D, we present results for tear film dynamics on eye-shaped domains. Our understanding of the tear film drainage system is modified by the role of the meniscus in driving flow on the 2D domain.

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MS35

Fluid Flow and Surfactant Transport in Models of Pulmonary Airway Reopening

Pulmonary airways are liquid-lined compliant tubes that convey gas to and from the alveoli, the primary site of gas exchange in the lung. Surfactant insufficiency results in airway closure and deranged pulmonary function. Fluid-structure interactions from airway reopening can significantly damage pulmonary tissue, and contributes to ventilation-induced lung injury. This talk will describe experimental and theoretical investigations of the physicochemical hydrodynamics of reopening that have been useful in identifying the damaging mechanical stimuli and may lead to protective methods of ventilation.

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MS35

Stability of Traveling Waves in Thin Liquid Films with Surfactant

A thin liquid film traveling down an inclined plane under the influence of gravity and surfactant is modeled in the lubrication approximation by a fourth order system of PDE equations. Stability of a novel traveling wave is explored through a dispersion relation and using the Evans function in one dimension; long-wave asymptotics describe the destabilizing effect of disturbances in two dimensions.

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MS35

Planar Extensional Motion of an Inertially-driven Liquid Sheet

The linear stability of an inertially-driven liquid sheet to symmetric perturbations is examined. For axial perturbations, viscous and inviscid sheets are asymptotically marginally stable, though transient growth can have an important effect. For transverse perturbations, inviscid sheets are asymptotically unstable to all wavelengths while viscous sheets are unstable to longwaves. For two-dimensional perturbations, inviscid sheets are unstable to all wavelengths and viscous sheets are asymptotically unstable to longwave transverse perturbations for any finite capillary number.

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MS36

Exascale Analytics of Massive Social Networks

Combinatorial techniques are proving useful in solving real-world challenges in traditional and emerging computational sciences such as chemistry, biology, and medicine, as well as applications in national security. Emerging real-world applications can be modeled using algorithms that process massive spatio-temporal complex networks, such as power grid stability, inference of gene function in protein interaction networks, and cancer research, as well as homeland security and national defense. In this talk we focus on the analysis of massive social networks using graph theoretic techniques. Our experimental studies use real-world graph instances with billions of elements and demonstrate superior performance on highly parallel systems such as the Cray XMT multithreaded architecture and the Sun's Niagara 2 Maramba system. We will also describe SNAP (Small- world Network Analysis and Partitioning), an open-source graph framework that we have developed for the exploration of massive complex networks and present new ideas on the exploration of the dynamic structure of massive spatio-temporal networks with billions of entities, such as understanding the genesis and dissipation of communities, allegiance switching, and source detection.

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MS36

Parallel Combinatorial BLAS and Applications in Graph Computation

Graph computations are difficult to parallelize using traditional approaches due to their irregular nature and low operational intensity. Many graph computations, however, contain sufficient coarse grained parallelism that can be uncovered by using the right set of abstractions. We have been developing a parallel combinatorial BLAS that consists of a small but powerful set of linear algebra primitives. We will explain our software design philosophy and report on the initial results with our reference implementation.

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MS36

Graph Detection Theory for Power Law Graphs

Detecting items of interest from the patterns of interaction in large graphs is the goal many graph analysis techniques. The basis of detection theory is computing the probability of a "signature' with respect to a model of the "background' data. Hidden Markov Models represent one possible signature model for patterns of interacation in a graph. Likewise, Kronecker graphs are one possible background model for graphs. Combining these models results in a filter that can be used compute the probability that a given graph contains a particular signature.

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MS36

Scaling up Graph Algorithms on Emerging Multicore Systems

Graph algorithms on sparse random networks typically suffer a 3-5X drop in performance when their memory footprint gets larger than the last-level cache on current systems. We attempt to ameliorate this drop for breadth-first search, and present several strategies to limit the number of non-contiguous memory references incurred in graph traversal. We extend these ideas to improve parallel scaling on cache-based multicore systems, by utilizing the shared and private caches more effectively, and by reducing synchronization overhead. We observe that the strategies discussed for breadth-first search are applicable to a large class of graph algorithms, and present another case study of a cache-aware parallel betweenness centrality algorithm for small-world networks.

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MS37

Anisotropic Bone Loss Characterized using Fabric-based Poroelasticity

Abstract unavailable at time of publication.

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MS37

Fabric Dependence of Poroelastic Wave Propagation

Abstract unavailable at time of publication.

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MS37

Quantitave Ultrasound of Bone: Bone Properties Conveyed by the Signal and Strategies for Inverse Solutions

Reliable quantification of microstructural and mechanical bone properties remains an open issue with relevance for the diagnosis of bone quality disorders, such as osteoporosis. The reconstruction of such parameters from nondestructive testing based on ultrasound testing and model-based solution of the identification inverse problem have been suggested by several investigators as novel techniques with high potential not only due to the reduced cost and its non-ionizing nature, but for the direct relationship and sensitivity of the propagation characteristics estimates to relevant bone properties that determine mechanical strength, which defines the ultimate criterion for diagnosis. To date, several procedures have been explored to inverse ultrasonic data acquired separately in transmission or in backscatter mode. Our group has reported in the past a method to estimate trabecular thickness from ultrasound backscatter measurements assuming a weak scattering model. Although a close agreement was obtained on average between predictions and the reference values, a modest predictability only was found at the individual level, suggesting that the model must be further improved before it can be translated to clinical applications (Padilla et al., Ultrason Imaging. 2006). Recently approaches taking advantage of the poroelastic nature of cancellous bone have been developed. These approaches assume that the Biot theory is a valid model of wave propagation and are aiming at either (i) recovering the properties of the fast and slow waves or (ii) directly reconstructing the bone properties that govern Biots theory. Results of inversion obtained in a set of human femoral condyles using approaches such as the Bayesian probability theory (Marutyan et al. J Acoust Soc Am. 2007) or a genetic algorithm will be presented. Because in many instances, the fast and slow waves overlap in the time domain and interfere, methods for an accurate estimates of their individual characteristics (i.e., amplitudes and velocities), are particularly useful to understand how these characteristics are influenced by strength-related bone properties. Finally, these developments offer a useful framework to assess to what extent the Biot theory assumed in the model is valid, and if any corrections can be suggested to overcome inconsistencies.

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MS37
Modeling Ultrasound Scattering from Cancellous Bone

Ultrasound scattering from cancellous bone arises from acoustic impedance mismatches between mineralized trabeculae and marrow. Because of the complex structure of the mineralized network, simplifying assumptions are often made to make models tractable. Despite these simplifying assumptions, several models have been shown to accurately predict frequency-dependent backscatter coefficients consistent with measurements from cancellous bone in vitro.

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MS38
Using Cilk++ to Multicore-Enable C++ Code

Cilk++ allows legacy C++ applications to be multicore-enabled by embedding a handful of keywords in the program source. The Cilk++ compiler and runtime platform work together to offer outstanding performance. In addition, the Cilkscreen race detector guarantees to find race bugs in ostensibly deterministic executions, thereby ensuring software reliability. To cope with legacy codes containing global variables, Cilk++ supports "hyperobjects" which allow races on nonlocal variables to be mitigated without lock contention or restructuring of code. This talk will overview the Cilk++ technology and how it can be used to multicore-enable applications.

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MS38
OpenMP: Addressing the Multicore Programming Problem with Established APIs

Abstract unavailable at time of publication.

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MS38
Intel Threading Building Blocks

Intel® Threading Building Blocks (Intel® TBB) is a commercially supported open-source C++ template library for multi-core programming. TBB lets you express logical parallelism, such as parallel loops, without becoming entangled in low-level threading details. TBB stresses nested parallelism, which is critical for modular software. TBB's concurrency-friendly containers simplify common patterns of sharing between parallel activities. TBB rounds out its concurrency support with critical low-level components such as locks, atomic operations, and a scalable memory allocator.

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MS38
Panel: Challenges of Multicore-Enabling Numerical Applications

Multicore processors are already ubiquitous. But the standard languages for writing technical programs are only beginning to adapt to this revolutionary change in the hardware platforms that run them. For FORTRAN, C, and C++, we need a minimally invasive, maximally portable, usable, and highly efficient way to extend the semantics to support parallel programming with high programmer productivity. The panelists, each expert in one of the competing approaches, will "square off" to discuss the issues confronting researchers and businesses who wish to produce multicore-enabled numerical software.

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MS39
Optimization of Transmission Spectra through Periodic Aperture Arrays

Periodic arrays of apertures in highly conductive materials are finding increasing application as frequency selective filters of electromagnetic waves, among other things. Such structures often exhibit pronounced peaks and dips in transmission at various frequencies, due to what are typically identified as resonances. We investigate an optimization strategy for finding appropriate material patterns to give desired transmission spectra, under various assumption on the medium and on the incoming radiation.

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MS39
Resonances of Thin Photonic Membranes

Consider the problem of calculating resonance frequencies and radiative losses of an optical resonator. The optical resonator is in the form of a thin membrane with variable dielectric properties. We report on our investigations using two very different approaches for doing such calculations [Gopalakrishnan, Moskow, and Santosa, Asymptotic and numerical techniques for resonances of thin photonic structures, SIAM J.Appl.Math., 69 (2008), pp.37-63]. The first is an asymptotic method which exploits the small thickness and high refractive index of the membrane. We derive a limiting resonance problem as the thickness goes to zero, and for the case of a simple resonance, find a first order correction. The limiting problem and the correction are in one less space dimension. This dimensional reduction makes this approach very efficient computationally. We show theoretical convergence estimates for the asymptotic problem.

The second approach, based on the finite element method with a truncated perfectly matched layer is not restricted to thin structures. While the asymptotic method finds resonance by solving a dense, but small, nonlinear eigenvalue problem, the finite element method yields a large, but linear and sparse generalized eigenvalue problem. For a specific photonic structure considered previously by others, we show that both the above methods reproduce a localized defect mode with a high quality factor, found earlier by finite difference time domain methods. We demonstrate the use of our new methods in numerical calculations, further illustrating their differences and advantages.

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MS39
The Inverse Born Series for Diffuse Waves and its Application to Optimal Tomography

Abstract unavailable at time of publication.

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MS39
Paper Parameter Estimation using Terahertz Time-domain Spectroscopy

Abstract unavailable at time of publication.

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MS40
Recovery of High Order Accuracy via Gegenbauer Reconstruction in Radial Basis Function Approximation for Discontinuous Problems

Radial basis function (RBF) methods have recently been investigated for solution of time dependent PDEs. These methods are mesh-free and yield high order accuracy if the function is smooth enough. The RBF approximation for discontinuous problems, however, deteriorates its high order accuracy due to the Gibbs phenomenon. In this talk we show that high order accuracy can be recovered from the RBF approximation contaminated with the Gibbs phenomenon if a proper reconstruction method is applied.

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MS40
Modeling of Storm Mergers and Tornadogenesis

Using the Advanced Regional Prediction System (ARPS), a numerical modeling software, we are investigating tornadogenesis promoted by storm mergers. The computer model output provides very detailed information about variables such as trajectories of air parcels, cold pools and origins of low-level vorticity. These can be viewed using the 3-d visualization tool Vis5d. Radar data of storm mergers and case studies are used to compare with our model output.

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MS40
Mathematically Modeling the Mass-Effect of Invasive Brain Tumors

When developing accurate models of tumor development, it is important to account not only for the invasion of tumor cells into healthy tissue, but also the resulting tissue damage (mass-effect). Intended to improve existing models of tumor invasion, the model presented here operates on a two-dimensional (2D) domain and uses continuum mechanics and finite element analysis to predict the mass-effect of an invasive tumor in heterogeneous brain tissue as a result of peri-tumor edema.

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MS40
Invisibility Cloaks for Asymmetric Objects

Metametrials have been constructed to create an “invisibility cloak” around an object. These work by guiding light rays around an object, letting them emerge on the opposite side as if the rays went straight through. To ensure the ray tracing used to compute the cloak is not the consequence of symmetry, we used Hamiltonian ray tracing to compute rays passing through cloaks of objects composed of parts of cones, cylinders, and spheres.

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MS40

Numerical Methodology for Fluid-structure Interaction Problems in Biological Systems

We consider the modeling and analysis of a fluid-structure interaction problem. The fluid equations, which are coupled through the boundary with an elastic structure, are studied using finite difference methods. Linear and nonlinear models will be considered in this study. Stability and convergence of the numerical methods will be presented. The numerical solutions will be compared against exact solutions, obtained using analytical tools such as Laplace Transforms. Applications of the model studied to intracranial saccular aneurysms will be presented.

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MS40

Detecting Complex Singularities in Two and Three Dimensions

An interesting phenomena in interfacial fluid flow is singularity formation. This can often be understood by analytically extending variables and equations to the complex plane C, and analyzing the motion of singularities in C. Numerical methods for tracking complex singularities, based on the asymptotic decay of Fourier coefficients (for periodic functions) have only been developed for functions of a single variable. We present a new numerical method to trace complex singularities for functions of two and three variables.

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MS41

Understanding the Effects of Rapid Evolution on Predator-prey Interactions Using the Theory of Slow-fast Dynamical Systems

Theory about the interplay between ecological and evolutionary processes with comparable time scales has not kept pace with accumulating evidence. The disparity between experiment and theory is partially due to the high dimensionality of models that include both evolution and ecological dynamics. I present how slow-fast systems theory reduces system dimension and generates graphical techniques that predict and explain the new types of qualitative dynamics that can occur in predator-prey systems with rapid evolution.

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MS41

Adapting Optimal Control from a Simple Aggregated Model to an Individual-based Model

A fundamental question in invasion biology and wildlife management concerns the most effective methods to limit the spread of and to control a harmful population. The hypothesis we investigate is whether optimal control theory applied to an aggregated, analytic model can be used to effectively control a harmful species modeled by an IBM, or whether interactions between individuals, their spatial distribution, and landscape heterogeneities limit effectiveness of the control methods derived from the aggregated model.

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MS41

Effect of the Three Dose Nature of the HPV Vaccine on HPV Spread

In recent years an HPV vaccine has been developed to curb HPV rates and therefore cervical cancer rates in women. The vaccine is administered in three doses, with increasing time in between doses. In this work we examine how hypothetical partial immunities and sequence failure rates affect the effective success rate of the vaccine on HPV spread and cervical cancer rates in a population.

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MS41

In-host Dynamics of Infectious Wildlife Disease: Mycoplasma Gallisepticum in Wild Finches

Since the early 1990s, bacterial conjunctivitis (Mycoplasma gallisepticum) in wild house finches (Carpodacus mexicanus) has been studied as a model wildlife disease system, providing opportunities to study disease at the individual, population and community levels. Here I present a dynamic model of an individual host's non-specific and specific immune responses to infection, with applications to both natural and controlled experimental infections.

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MS42

Lubrication Models of Langmuir Foams

Langmuir layers are molecularly-thin polymer layers on a fluid surface. They exhibit multiple phases (fluid, gas, liquid crystal, isotropic or anisotropic solid); line tension drives the system to minimize the phase boundary's perimeter. Langmuir foams - bubbles of one phase separated by thin lamellae of a second phase - are experimentally ubiquitous. The gradient flow drives these lamellae to thin and sometimes rupture. We model this thinning via lubrication theory for a Hele-Shaw model problem, and for fluid-fluid and fluid-gas Langmuir foams.

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MS42
Diffuse Interface Modeling of Electrowetting Drops

Electrowetting has recently been explored as a mechanism for moving small amounts of fluids in typical confined spaces. Here we develop a diffuse interface model for drop motion, due to electrowetting, in a Hele-Shaw geometry. We show that details of the contact angle significantly affect the timescale of motion in the model. The shape dynamics and topology changes in the model agree well with the experiment.

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MS42
Particle Migration and Instabilities in Inclined Plane Flow of Particle-laden Thin Films

A theory is formulated in order to describe the dynamics of a thin particle-laden film flowing down an inclined plane. The evolution of particle concentration is modeled by taking into account the shear-induced migration of particles. A pair of coupled PDEs governing the film height and particle concentration is derived using lubrication approximation. A numerical code for solving the governing system is developed and the results are compared to preliminary experimental data.

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MS42
Electrically Driven Squeezing of a Droplet Between Plane-parallel Surfaces

Abstract unavailable at time of publication.

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MS43
Scalable & Efficient Parallelization of Graph Methods for Boolean Satisfiability and Power Grid Analysis on the Cray XMT

Graph-based algorithms have a broad applicability to many different areas of science and technology. Unfortunately, executing them efficiently for large-scale graphs requires a significant time and resource investment on traditional HPC systems. The Cray XMT multithreaded architecture provides specialized hardware designed for the efficient parallel execution of highly irregular codes, such as those derived from graph algorithms. This presentation will discuss our experiences in implementing two graph-based algorithms on the Cray XMT system: a Boolean satisfiability solver based on parallel Survey Propagation and an exact, edge-based, weighted Betweenness Centrality calculation applied to power grid analysis.

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MS43
Novel Graph Algorithms for Structure Extraction from Informatics Networks

Large informatics graphs such as large social and information networks that are increasingly common in Internet and high-performance computing applications have surprising complex and subtle structural and dynamic properties. For instance, their size alone, which can be in the millions or billions or more of nodes, immediately renders many traditional algorithmic tools unusable. In addition, their extreme sparsity and adversarial noise properties render many existing statistical tools inappropriate. Finally, due to their heavy-tailed properties, these networks are not meaningfully low-dimensional nor are they meaningfully high-dimensional, and thus methods that explicitly or implicitly rely on either of those common assumptions have severe limitations. I will describe recently-developed algorithms that begin to deal with some of these problems and that allow the analyst to probe in very fine ways nontrivial structural properties of extremely large informatics networks. Examples of these algorithms include generalizations of spectral graph partitioning to find good cuts that are near a specified node, efficient methods to compute graph resistances that can be used to identify dispro-

portionately important or influential nodes, graph partitioning algorithms that interpolate between spectral and flow-based algorithms, and heuristics to characterize the large-scale clustering structure of large networks.

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MS43

Parallel Implementation of Tensor Decompositions for Large Data Analysis

Large data sets can often be mapped into multidimensional arrays, which we call tensors; the resulting tensor is usually extremely sparse. Similar to the SVD decomposition of a matrix there are a number of proposed tensor representations in terms of factors. This talk will describe serial and parallel implementations of several algorithms for tensor analysis, in particular algorithms which compute PARAFAC and Tucker representations of tensors. We will discuss previous and potential applications of these representations.

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MS44

Cancellous Bone Interrogation Using Upscaling

This paper considers the application of multiscale FEM to the modeling of cancellous bone as an alternative for Biots model, whereby the main intention is to decrease the extent of the necessary laboratory tests. At the beginning the paper gives a brief explanation of the multiscale concept and thereafter focuses on the modeling of the representative volume element (RVE) and on the calculation of the effective material parameters including an analysis of their change with respect to increasing porosity. The latter part of the paper concentrates on the macroscopic calculations, which is illus- trated by the simulation of ultrasonic testing and a study of the attenuation dependency on material parameters and excitation frequency. The results endorse conclusions drawn from the experiments: increasing excitation frequency and material density cause increasing attenuation. The homogenization of a poroelastic structure will also be considered using two-scale-stochastic convergence. The effective equations will be derived.

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MS44

Clinically Relevant Parameter Estimation: What Parameters Should the Mathematical Model for Wave Propagation in Cancellous Bone Include?

The bone research community has developed a unique nomenclature for the set of parameters that describe the morphometry of trabecular bone as extracted from histological, microCT, and high resolution MR images. This terminology differs significantly from those found in the theories of random heterogeneous media and homogenization. In order to facilitate acceptance of new parameters extracted from mathematical models of wave propagation in trabecular bone, some care must be exercised in the choice of parameters and education of clinicians as to these new quantitative methods. In this presentation, I will review the relationship between existing parameters and suggest targets for future clinical relevance.

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MS44

Dehomogenization with Application in Ultrasound Probing of Cancellous Bones

Dehomogenization refers to the process of inferring from macroscopic measurement the micro-architectural information. l will start with simple examples and elaborate on how this can be applied to iultrasound probing of cancellous bones.

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MS44

Mesoscale Dynamics of Discrete Models of Bone Tissue

We address the problem of efficient simulation of deformation and wave propagation in bone tissue, in particular cancellous bone. Non-linear nature of the microscale constitutive equations and disordered microstructural geometry make homogenization less effective, or even impossible to apply. We propose an alternative approach: a dimension reduction strategy for discrete microstructural models. This strategy produces equations of balance for average density, momentum and energy at any mesoscopic space and time scales. The main difficulty, as in homogenization, is to find closure for these balance equations. We present some new ideas on how to obtain an approximate closed system for modeling mesoscopic continuum. The proposed approach is based on space-time averaging and concentration inequalities from probability theory.

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MS45

An A Posteriori Analysis of Finite Volume Element Method for Quasi-linear Elliptic Problem

We introduce and analyze two computable error estimators for finite volume element solution of a quasi-linear elliptic problem: residual type and post-processing type.

The residual error estimator amounts to upper and lower bounds of the error in certain norm. Moreover, the post-processing type error estimator is based on the superconvergence of the numerical solution. Numerical experiments will be presented to illustrate the performance of the proposed estimators. This is a joint work with Dr. Chunjia Bi at Yantai University in China.

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MS45

FVM for a Biosensor Model Using Nonlocal PDEs

FVM is considered for a system of nonlinear PDEs coupled with ODEs defined only on a portion of the domain boundary. Under certain assumptions, the existence, uniqueness, and asymptotic to the steady-states are considered. A sub-optimal error estimate is given along with numerical examples.

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MS45

Error Estimation for a Cartesian Grid Finite Volume Method for Diffusion Problems with Discontinuous Coefficients

Diffusion operators with discontinuous coefficients are encountered in problems such as heat conduction and subsurface flow. Accurate discretization is challenging when the discontinuities are not grid-aligned. We describe a Cartesian grid finite volume method that represents interfaces with cut cells and models effective diffusion coefficients near the discontinuity with an optimal projection scheme. This is coupled to an adjoint-based scheme that can be used to provide reliable error estimates and to refine the model representation.

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MS45

A Posteriori Error Analysis of Finite Volume Methods with Applications to Elliptic, Parabolic and Navier-Stokes Equations

The goal-oriented a posteriori error analysis based on duality and adjoint operators is carried out in our work for finite volume methods for ellitpic, parabolic, and Navier-Stokes equations. The analysis is based on an equivalence between a cell-centered finite volume scheme for each problem and the corresponding lowest order mixed method with proper quadrature rules. The error in the name of quantity of interest is then computed exactly as a linear functional.

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MS46

Solitary Wave Dynamics in a Slowly Varying Potential

We study the Schrodinger equation with Hartree nonlinearity, with a slowly varying smooth potential, $V(x) = W(hx)$, and with an initial condition which is ϵ away in H^1 norm from a soliton. We show that up to time $\log(1/h)/h$ and errors of size $\epsilon + h^2$ in H^1, the solution is a soliton evolving according to the classical dynamics of a natural effective Hamiltonian, which we compute explicitly. This result is based on methods of Holmer-Zworski, who prove a similar theorem for the Gross-Pitaevskii equation, and on spectral estimates for the linearized Hartree operator recently obtained by Lenzmann.

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MS46

A Reformulation and Applications of Interfacial Fluids with a Free Surface

The classic water wave problem consists of finding the irrotational evolution of an ideal fluid with a free interface, subject to gravity. In this talk, we present a recent reformulation of water wave, given in terms of a nonlocal equation that connects the free interface and the velocity potential evaluated on the free interface. We also present an extension of this nonlocal formulation to interfacial fluids bounded by a free surface, and discuss applications of these equations to the study of interfacial solitary waves. Of particular interest is an asymptotically distinguished (2+1)-dimensional generalization of the intermediate long wave equation, which includes the Kadomtsev-Petviashvili equation and the Benjamin-Ono equation as limiting cases. Lump-type solutions to this (2+1)-dimensional ILW equation are obtained, and the speed versus amplitude relationship is shown to be linear in the shallow, intermediate, and deep water regimes.

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MS46

Multidimensional Solitons with Compact Support

Solitons for quasilinear integrable dispersive equations, such as the Fermi-Pasta-Ulam and Korteweg-de Vries equations, all have infinite support. That is, although the solitons are localized in space, they only decay asymptotically to zero. Recently, (with Philip Rosenau) we discovered a general class of nonintegrable equations supporting solitons in one, two, and three dimensions with compact support, called compactons. In contrast to the usual solitons, these compactons are identically zero outside a central core region, are nonlinearly self-stabilizing and exhibit the remarkable soliton property that after colliding with other compactons, they re-emerge with the same coherent shape. Also, compact initial data decomposes into a train of compactons. That is, compactons behave similarly to solitons associated with completely integrable PDEs.

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MS46

Computation of Time-periodic Solutions of Nonlinear PDE

I will describe a spectrally accurate numerical method for finding non-trivial time-periodic solutions of nonlinear PDE. We minimize a functional (of the initial condition and the period) that is positive unless the solution is periodic, in which case it is zero. We solve an adjoint PDE to compute the gradient of this functional with respect to the initial condition. We apply our method to the Benjamin-Ono equation and the vortex sheet with surface tension.

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MS47

On the Local/global Median Phenomenon in Stable Matchings

About a decade ago, Teo and Sethuraman showed that there is a stable matching that matches each participant to his (lower or upper) median stable partner. Such a stable matching turns out to be not only fair in a local sense but also in a global sense. In particular, we will show that the set of stable matchings of I form a median graph $G(I)$, and the said stable matchings are medians of $G(I)$.

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MS47

The Genus of a Digital Image is Determined by its Foreground, Background, and Reeb Graphs

Our main result is that the topological genus of the boundary of a digital image (itself a topological surface) is precisely half of the sum of the cycle ranks of three particular graphs: the "foreground graph" and "background graph," which capture topological information about the digital image and its complement, respectively, and the Reeb graph, relative to the natural height function, associated with the digital image's boundary. Additional results include a characterization of when the cycle rank of the Reeb graph fails to equal the genus of the digital image's boundary (which can happen by virtue of the failure of the natural height function on the boundary of the digital image to be a Morse function).

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MS47

Sharing the Cost of a Capacity Network

We consider a communication network where each pair of users requests a connection guaranteeing a certain capacity. The cost of building capacity is identical across pairs. Efficiency is achieved by any maximal cost spanning tree. We construct cost sharing methods ensuring Stand Alone core stability, monotonicity of one's cost share in one's capacity requests and continuity in everyone's requests. We define a solution for simple problems where each pairwise request is 0 or 1, and extend it piecewise-linearly to all problems. The Uniform solution obtains if we require one's cost share to be weakly increasing in everyone's capacity request. In the BHM solution, on the contrary, one's cost share is weakly decreasing in other agents' requests. The computational complexity of both solutions is polynomial in the number of users. The Uniform solution admits a closed form expression, and is the analog of a popular solution for the minimal cost spanning tree problem.

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MS47

On Decomposition Trees of k-trees Representable as Unit-Rectangle-Visibility Graphs

For k = 1,2,3, let UDT(k) denote the set of decomposition trees of k-trees that are representable as unit rectangle-visibility graphs. Using known characterizations of trees in UDT(1) and in UDT(3), we establish the relationship between the latter two sets and with the uncharacterized set UDT(2).

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MS48

Bounds and Error Estimates for Resonance Problems

Abstract unavailable at time of publication.

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MS48

Controlling Dispersion Relations of Frequency Dependent Materials near Resonance

Abstract unavailable at time of publication.

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MS48

The Exterior Cloak

We will introduce a new cloaking strategy for conductivity and Helmholtz equations. Our cloak has the advantage that, while maintaining a very good accuracy, it does not use exotic materials. Numerical results to suport the analysis will be presented.

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MS48

Sensitivity Analysis of Scattering by Open Dielectric Waveguides

Abstract unavailable at time of publication.

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MS49

European Option Pricing for Inventory Management and Control

We explore the use of option contracts as a means of managing and controlling inventories in a retail market. Specifically merchants can buy option contracts on unsold inventories of retail goods as a method for managing, pooling, or transferring risk. We propose and price a new class of European put options on an inventory where the buyer is allowed to freely control the sale price of the underlying good during the contract period.

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MS49

A Stochastic Approach to Modeling Acid Precipitations Impact on a Tri-trophic Aquatic Ecosystem

We implemented an empirically-based Markov Chain to model variable environmental conditions of an acidified lake. Simulations were run to represent a given time frame of varying conditions that may impact ecosystem dynamics. The simulation results were then compared with a deterministic approach using optimal environmental conditions as well as the mean environmental conditions from the stochastic model.

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MS49

Kinetic Modeling of the Maillard Reaction

The Maillard reaction is a complex sequence of chemical reactions involving amino acids and sugars. It plays an important role in aging, and contributes to the pathogenesis of diabetes and neurological diseases such as Alzheimer's. In this talk a model for the Maillard reaction is presented. The analysis of the resulting system involves a combination of analytic methods and numerical simulations. The results from this analysis will be compared with experimental data for the Maillard reaction.

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MS49

Vaccinating Against HPV in a Dynamical Social Network

We develop a dynamical network model to examine the relative merits of strategies for vaccinating women against the sexually transmitted Human Papillomavirus, which can induce cervical cancer. The model community is represented as a sexual network of individuals with links dynamically created and destroyed through statistical rules based on the node characteristics. Various strategies for distributing an allotted number of doses of vaccine are tested for effectiveness in reducing the incidence of cervical cancer.

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MS49
Meteorologically-Adjusted PM-fine Trend Analysis

Fine particulate matter (PM2.5) is a complex mixture of solid and particles suspended in the air that have an aerodynamic diameter of 2.5 micrometers or less. These particles can impose a variety of harmful health effects. The purpose of this project was to evaluate the effectiveness of EPAs NOx-SIP Call (Nitrogen Oxides State Implementation Plan Call) in curbing PM2.5 concentrations in North Carolina. Autoregressive linear modeling techniques were used to remove the effects of meteorology.

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MS49
Pricing of American Inventory Options

We expand our work on option pricing in a retail setting to include American-type contracts, where the retailer can exercise the option at any time during the contract period, thus requiring that the writer pay for, and remove, any unsold inventory. This twist to our previous work adds a layer of complexity to the pricing problem, but also makes it more realistic, whereby the retailer can dump low selling goods immediately.

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MS50
A Discontinuous Galerkin Solver for Full-band Boltzmann-Poisson Models

We present new preliminary results of a discontinuous Galerkin (DG) scheme applied to deterministic computations of the transients for the Boltzmann-Poisson (BP) system describing electron transport in semiconductor devices. We use the full band models, which guarantee accurate physical pictures of the energy-band function. These models are widely used in DSMC simulators, but only recently the transport Boltzmann equation was considered, where approximate solutions were found by means of spherical harmonics expansion of the distribution function. The DG method allows us to consider these more complex band structure models without sacrificing computational efficiency. We use energy band data to obtain a smooth interpolant of the energy band function to test our DG solver in the case of bulk silicon. More general applications will be considered in the future.

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MS50
Lagrangian Simulations of the Vlasov Poisson System

In the Vlasov Poisson system, the ratio of the electron time scale to the ion time scale is at least 10^4, making this a stiff system. In this talk we will investigate the use of high order time stepping, based on integral Differed Correction, as a way of increasing efficiency in fully lagrangian simulations of the Vlasov Poisson system. The goal is to explore ways of bridging the electron ion time scale. We apply the method to several test case, including the virtual cathode and two stream instability.

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MS50
Lagrangian Particle Method for the Vlasov-Poisson Equations

A numerical method is presented for collisionless electrostatic plasmas based on the Lagrangian form of the Vlasov-Poisson equations. The charge flow map is represented by quadrilateral panels in phase space. The particle-particle force is regularized and the panels are adaptively subdivided to resolve filamentation. Simulations are presented for the instability of an electron beam.

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MS50
Conservative High Order Semi-Lagrangian Method for the Vlasov Equation

We propose a novel semi-Lagrangian method for the Vlasov equation, which combines Strang splitting in time with WENO reconstruction in space. A key insight is that the spatial interpolation matrices, used in the reconstruction process, can be factored into flux matrices, because of which WENO can be applied. The CFL time step restriction is removed in the semi-Lagrangian framework. The quality of the method is demonstrated by several classical problems in plasma physics.

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MS51

Approximate Cloaking and Applications

Less-than-ideal cloaking structures, in addition to being more physically realistic than ideal ones, may be useful in the trapping and manipulation of waves. I will describe joint work with M. Lassas, Y. Kurylev and G. Uhlmann on approximate cloaks for a class of equations containing the acoustic and Schroedinger wave equations, and their possible applications.

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MS51

Virtual Reshaping and Invisibility in Obstacle Scattering

In this talk, we consider reshaping an obstacle virtually by using transformation optics in acoustic and electromagnetic scattering. Among the general virtual reshaping results, the virtual minification and virtual magnification are particularly studied. Stability estimates are derived for scattering amplitude in terms of the diameter of a small obstacle, which implies that the limiting case for minification corresponds to a perfect cloaking, i.e., the obstacle is invisible to detection.

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MS51

Cloaking by Anomalous Localized Resonance: Principles, Problems and Possibilities

We discuss the mechanism for cloaking or hiding of objects from detection by probing with electromagnetic waves using the mechanism of anomalous localized resonance, also called reactive cloaking to distinguish it from the alternative method based on transformation optics or refraction. We highlight the requirements for this type of cloaking, and compare them with those of refractive cloaking. We discuss the challenge common to both methods of achieving cloaking over extended spectral ranges and spatial regions, and possible ways of meeting the challenge.

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MS51

Approximate Cloaking by Change of Variables

In this talk we will discuss about the possibility of cloaking materials from monochromatic EM guided waves or acoustics waves using only nonsingular (regular) cloaks. Although perfect cloaking is impossible using only regular materials, we will describe the procedure of building an approximate cloak which achieves cloaking within a certain error independent of the materials to be cloaked. Two central ideas behind our results are: (i) the use of a suitable nonsingular transformation of variables, and (ii) the introduction of a suitable conducting layer around the material to be cloaked in between the material and the cloak. We will introduce the main ideas and the analytical results of our work and will present several numerical results for the two and three dimensional case, complementary to our analysis, to highlight the role of the conducting layer and the role of the cloak in the cloaking process, and to show how the error in the approximate cloaking depends on the conductivity in the layer. In all our numerical results extremely singular materials (analytically described) to be cloaked will be considered. We will also present the analytical arguments used to obtain such materials and will numerically highlight their singular behavior. Numerical examples will be discussed showing the approximate cloaking achieved using these methods.

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MS52

Correctors, Homogenization, and Field Fluctuations for the $p_\epsilon(x)$-Laplacian with Rough Exponent

In this talk, properties of local fields inside mixtures of two nonlinear power law materials are studied. This constitutive model is frequently used to describe several phenomena ranging from plasticity to optical nonlinearities in dielectric media. We develop new multiscale tools to bound the local singularity strength inside microstructured media in terms of the macroscopic applied fields.

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MS52

A Homotopy Method in Regularization of TV Minimization Problems for Image Denoising

Homotopy methods can often be used to make mathematical programming problems easier to solve. One source of notoriously difficult problems is total variation image denoising problems. We present a method using the regularization parameter as a homotopy parameter to numerically approximate solutions to TV minimization problems. A relationship is established between the homotopy parameter and the radius of the Kantorovich ball guaranteeing the convergence of Newton's method. Convergence analysis and numerical results are presented.

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MS52

The Mathematics Behind Energy and Earth Systems Modeling

Our use of energy and the resulting effects on the worlds climate are tightly interwoven. Global warming effects are already having a clear impact, including melting polar ice caps, hurricanes and other extreme events. In this talk, I will give a short history of some of the mathematical foundations behind these models and discuss the connections between mathematics, the development of new and efficient energy sources and methods for analyzing the effects of climate change.

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MS52

Modeling Faculty Teaching Workload as a Linear Program and Automating

We model the problem of assigning classes to faculty as a linear program, which consists of approximately 8000 variables and 450 equality and inequality constraints for the Department of Math at UTPA. Moreover, we describe the use of the modeling language GAMS, which facilitates writing large problems. Finally, we show a web application created by students to automate many of the processes.

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MS53

Models for Superspreading Micro-droplets

Many fluid thin-films contain surfactants, and moreover at such concentrations that micellar aggregates form within the fluid. This talk will discuss recent models for this aggregation and how their presence affects the surface tension. On small scales Marangoni forces, created by surface tension gradients, become important and for some classes of surfactants "superspreading" occurs. This will be discussed in the light of recent modelling.

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MS53

Bistability in Liquid Crystal Displays

Motivated by applications in the Liquid Crystal Display (LCD) industry, we consider a thin film of nematic liquid crystal (NLC) sandwiched between parallel plates. NLC molecules can rotate the plane of polarized light, so when placed between crossed polarizers, light may pass through the NLC layer if the molecules are suitably oriented. We consider a new design for a bistable LCD, with distinct zero-field states; and investigate switching by transient application of an electric field.

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MS53

Coarsening of Dewetting Films 2: Transient and Self-similar Dynamics

Using the dynamical system model for the evolution of drops derived in the previous talk, we explore connections with mean-field models of coarsening, including the Liftshitz-Slyozov-Wagner model. While information is lost in the mean-field model, we show that they can give reasonable predictions of the self-similar distribution of drops sizes. However, before the system achieves self-similarity, significant transient dynamics can occur. We describe a "stair-stepping" mode that occurs in drop populations arising from spinodal dewetting.

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MS53

Coarsening of Dewetting Films I: the Influence of Gravity

Dewetting instabilities for thin films of viscous fluids yield arrays of droplets. The PDE model given by lubrication theory is reduced to a dynamical system for the evolution of the drops. The number of drops successively decreases as smaller drops are eliminated. While gravity has a very weak influence on the original film, we show that it has a significant influence on the later stages of the dynamics, dramatically slowing the rate of coarsening.

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MS54

Injective Colorings of Sparse Graphs

Let mad(G) denote the maximum average degree (over all subgraphs) of G and let $\chi_i(G)$ denote the injective chromatic number of G (in an injective coloring, vertices must receive distinct colors if they have a common neighbor). If Δ denotes the maximum degree of G, then clearly $\chi_i(G) \geq \Delta$. We study upper bounds on mad(G) that imply $\chi_i \leq \Delta + c$ for $c \in \{0, 1, 2\}$, obtaining the following results. If mad$(G) < \frac{14}{5}$ and $\Delta \geq 4$, then $\chi_i(G) \leq \Delta + 2$. When $\Delta = 3$, we show that mad$(G) < \frac{36}{13}$ implies $\chi_i(G) \leq 5$; in contrast, we give a graph G with $\Delta = 3$, mad$(G) = \frac{36}{13}$, and $\chi_i(G) = 6$. If mad$(G) \leq \frac{5}{2}$, then $\chi_i(G) \leq \Delta + 1$; similarly, if mad$(G) < \frac{42}{19}$, then $\chi_i(G) \leq \Delta$. When G is a planar graph with $\Delta \geq 4$, we have the following improvements. If girth$(G) \geq 9$, then $\chi_i(G) \leq \Delta + 1$; similarly, if girth$(G) \geq 13$, then $\chi_i(G) = \Delta$.

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MS54

Some Results on Ramsey Numbers and Turán Numbers

The Ramsey number $r(G, H)$ of two graphs G and H is the least n such that every red/blue edge-coloring of K_n contains either a red G or a blue H. The Turán number $ex(n, G)$ is the maximum number of edges in an n-vertex graph that does not contain G as a subgraph. The Ramsey problem and the Turán problem are related, and they play central roles in extremal graph theory. We first note a simple but useful connection between $r(G, K_m)$ and $ex(n, G)$, which can be used to generalize some known results. Then, among other things, we discuss $r(G, K_m)$ when G is a theta graph: that is G is obtained by joining two vertices with internally disjoint paths. We will also discuss the Turán numbers of subdivisions of cliques and the effect on $ex(n, H)$ when a "bridge' is added between two adjacent vertices of H.

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MS54

Multi-coloring the Mycielskian of Graphs

A *k-fold coloring* of G is a function assigning to each vertex a set of k colors so that adjacent vertices receive disjoint color sets. Let $\chi_k(G)$ be the minimum number of colors in a k-fold coloring, and let $\mu(G)$ be the Mycielskian of G. We conjecture that for any $n \geq 3k - 1$, there is some G with $\chi_k(G) = n$ and $\chi_k(\mu(G)) = n + k$. This is equivalent to proving $\chi_k(\mu(K(n, k))) = n + k$ for the Kneser graphs $K(n, k)$ with $n \geq 3k - 1$. We confirm this when k is 2 or 3 or divides n, and when $n \geq (3k^2)/(\ln k)$. Moreover, we determine the values of $\chi_k(\mu(C_{2q+1}))$ for $1 \leq k \leq q$.

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MS54

The Degree-associated Reconstruction Number of a Graph

The *reconstruction number* of a graph is the minimum number of one-vertex-deleted subgraphs needed to determine it. The *degree-associated reconstruction number* drn(G) is the minimum number needed when the degree of the missing vertex is given along with each subgraph. We characterize drn=1. Almost always drn≤2. For all but two caterpillars, drn=2. We know only two trees with drn>2, but drn≥3 for any vertex-transitive graph other than K_n or its complement. For an n-vertex k-regular graph, drn$\leq \min\{k + 2, n - k + 1\}$.

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MS55

Detecting Community Structure in Dynamic Networks

Community structure detection in networks has important applications in understanding social structures, spread of epidemics, etc. However most algorithms for detecting communities (defined as tightly connected group of nodes) are applicable only to a static network with fixed nodes and edges. In reality, social networks are dynamic and the connections change with time. In this talk, we present an algorithm that can dynamically detect the change in communities as the network evolves over time steps.

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MS55

High Performance Computing for Large Graph Problems

Graph abstractions have long been central to sparse matrices, parallel computing, chemistry, logistics and many other areas. But recent years have witnessed a further broadening of graph models to represent entities and relationships in ecology, social science, text analysis and other fields. There is a growing need for high performance graph algorithms to address problems in which the data is very large and/or timely response is important. For complex graphs, algorithms often exhibit very poor locality, and so cache-based architectures, and message-passing programming models deliver disappointing performance. In this talk, I will discuss our exploration of non-traditional architectures and programming models for graph algorithms, placing this work in the larger context of ongoing changes within the high performance computing universe.

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MS55

Anatomy of a Distributed Graph

For the large-scale matrix and vector data structures used in scientific computing the data distribution process has become relatively well understood. However, the increasing prominence of large-scale graph-based problems has magnified the importance of effective computation with distributed graph structures. Based on our experience with the Parallel Boost Graph Library, we present an overview of the unique characteristics of distributed graph data structures and the impact of these characteristics on application development and performance.

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MS55

Structure of Large Scale Social Contact Graphs and its Effect on Epidemics

In recent years, there has been a lot of interest in studying the spread of epidemics on social contact graphs. We discuss important structural properties of a class of large scale synthetic social contact graphs. We discuss what effect the underlying graph structure has on the disease dynamics, and how these structural properties can be used in designing effective interventions for epidemics (e.g., whom to vaccinate), which is an important public health issue.

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MS56

Implicitly Coupled Solvers for the Simulation of Fluid-Structure Interaction

Simulation of fluid-structure interaction is a complex problem that involves modeling different physics for the fluid and the structure and coupling them together in a stable and efficient manner. In this talk we discuss scalable techniques in the multilevel Newton-Krylov-Schwarz family for solving the nonlinear, monolithically coupled fluid-structure interaction system on moving finite element meshes in the arbitrary Lagrangian-Eulerian framework. We report numerical results obtained on supercomputers for the simulation of blood flows in arteries.

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MS56

Application of Newton-Krylov Methods to the Implicit Solution of Problems in Radiation Hydrodynamics

The fields of radiation and hydrodynamics are, individually, time-honored disciplines. However, only recently have complex problems in radiation hydrodynamics–a single field encompassing the interplay of radiation and hydrodynamics together–become computationally tractable. We discuss how we are using implicit nonlinear solvers, especially preconditioned Newton-Krylov methods, as solution techniques in this field. We also discuss the multiphysics, multimodel challenges we face: diverse distance scales, time scales, physical regimes, species, and radiation-matter couplings.

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MS56

Schur-Complement and Block-Preconditioned Iterative Techniques for Coupled Subsurface Flow and Geomechanics

In this work, we consider efficient solution methods for mixed finite element models of fluid flow through deformable porous media. Our main focus is preconditioning techniques to accelerate the convergence of Newton-Krylov solvers. We highlight an approach in which preconditioners are built from block-factorizations of the coupled systems. The resulting methodology allows one to extend efficient single-physics preconditioners to multi-physics applications, leading naturally to an object-oriented simulation approach.

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MS56

Nonlinear Solvers and Their Multiphysics Applications

This presentation provides an overview of issues arising in large-scale multiphysics simulations and general approaches for solutions. We discuss several popular implicit nonlinear solver technologies and show examples of uses of one of these, the Newton-Krylov method, within the context of multiphysics problems.

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MS58

Deterministic Uncertainty Quantification for Finite Volume Approximations of Systems of Nonlinear Conservation Laws

We consider the deterministic propagation of statistical model parameter uncertainties in numerical approximations of nonlinear conservation laws. Particular attention is given to finite volume discretizations of the Reynolds-averaged Navier-Stokes equations with (1) PDE turbulence models and (2) finite rate chemistry models for a nitrogen-oxygen atmosphere. As a practical matter, these calculations are often faced with many sources of parameter uncertainty. Some example sources of parameter uncertainty include empirical equations of state, initial and boundary data, turbulence models, chemistry models, catalysis models, radiation models, and many others. To deterministically calculate the propagation of model parameter uncertainty, stochastic independent dimensions are introduced, see for example [M. Klieber and T.D. Hien, The Stochastic Finite Element Method, John Wiley and Sons, 1992], [R.G. Ghamen, Ingredients for a General Purpose Stochastic Finite Element Formulation, CMAME, Vol. 168, 1999], or [D. Xiu and G. Karniadakis, Modeling Uncertainty in Flow Simulation via Generalized Polynomial Chaos, JCP, Vol. 187, 2002]. In the present formulation, piecewise polynomial basis representations are constructed in these new independent dimensions and the resulting discretized conservation law systems solved using a multilevel domain decomposition solution technique well suited to parallel computer architectures. Keen attention is given to situations arising in compressible flow computations whereby discontinuites in the solution variables occur in both physical and stochastic coordinates. This necessitates adaptive discretization via limiting in both physical and stochastic coordinates. Various numerical computations with statistical model parameter uncertainty are shown to demonstrate properties of the formulation:

- 2D and 3D compressible RANS flow with statistical turbulence model uncertainty.
- 2D and 3D compressible RANS flow with 5 species nitrogen-oxygen finite-rate chemistry model with statistically uncertain chemical reaction model parameters.

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MS58

Recent Developments of the Multiscale Finite Volume Procedure

The multi-scale-finite-volume procedure (MSFV, Jenny et. al, JCP 2003) for the approximated solution of elliptic problems with variable coefficients has been recently modified in various directions to cope with the requirements from different fields of applications. However, the key ideas of the MSFV procedure (see also Chen and Hou, JCP 2003) are shared by all developments. First, a set of basis functions honoring the fine-scale features of the variable coefficient are introduced to define a coarse scale problem with drastically fewer degrees of freedom. Second, the same basis functions are used to reconstruct a fine-scale solution after the coarse-scale problem has been solved. Finally, a vector field approximating the gradient of the solution and fulfilling the conservation law represented by the original elliptic equation can be evaluated. Recently introduced generalizations include an iterative procedure to improve the solution to any desired level of accuracy (Hajibeygi et al., JCP 2008; Bonfigli and Jenny, submitted JCP) and the application to parabolic problems (Hajibeygi and Jenny, submitted JCP). In the first part of the talk we present the basic concepts of MSFV with particular attention to its iterative version IMSFV. In the second and conclusive part we then provide an overview on currently considered applications. These include compressible and incompressible reservoir simulations governed by the Darcy's law, the simulation of incompressible flows around complex geometries solving the Navier-Stokes equations with the immersed-boundary approach, and the simulation of flows governed by the Stokes and Darcy equations in different parts of the integration domain.

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MS58

Immersed Finite-Element-Volume Methods for Interface Problems

We consider finite-element-volume methods based on immersed finite element (IFE) functions for 2nd order elliptic boundary value problems with discontinuous coefficients. The IFE basis functions are piece-wise linear polynomials satisfying the jump conditions approximately (or even exactly in certain situations) at the material interface. In addition, the mesh used in IFE does not have to be aligned with the interface. Therefore structured Cartesian meshes can be used in immersed finite-element-volume methods for solving problems with non-trivial interfaces. IFE based on triangular and rectangular meshes will be discussed and numerical examples will be presented to illustrate features of these methods.

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MS58

A Posterior Error Estimate for Finite Volume Methods of Second Order Elliptic Problems

We establish a posterior error analysis for finite volume methods of second order elliptic problems. The residual based error estimator can be applied to different types of finite volume methods.

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MS59

Advanced Numerical Modeling and Data Assimilation for Flood Management

Abstract unavailable at time of publication.

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MS59

In-situ and Remote Monitoring of Environmental Water Quality

Abstract unavailable at time of publication.

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MS59

Developing Operational Systems with DelftFEWS to Turn Available Data Streams into Information for Operational Water Management

Abstract unavailable at time of publication.

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MS59

Decision Support Systems for Integrated Water Resources Management

Abstract unavailable at time of publication.

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MS60

The Near Field Refractor Problem

Given an $n-1$ dimensional screen find an interface surface in R^n that separates two media with different index of refraction, say glass and air, such that all rays emanating from one point and with given intensity illuminate the screen with a prescribed intensity. We prove the existence of this surface. This yields a lens which focus all rays emanating from one point into a screen in a prescribed way.

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MS60

Integral Surfaces of Vector Fields and Optical Design

The problem of controlling a single ray bundle has applications to the design of both image formation systems and for illumination systems. Despite being fundamental to both these of these areas, the problem is still not fully understood. I will show how it is naturally framed in terms of constructing surfaces that are orthogonal to a collection of given vector fields and give several applications, including a driver-side mirror that has no blind-spot or distortion.

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MS60

Optical Design of Freeform Mirrors and Lenses for Beam Shaping

Two-mirror and two-lens devices converting an incident plane wave of a given cross section and intensity into an output plane wave irradiating at a given set with prescribed intensity are required in many applications. Most of the known designs are restricted to rotationally symmetric mirrors/lenses. In this talk I will discuss designs with freeform mirrors/lenses. It will be shown that these problems can be studied and solved numerically as optimal transportation problems with Fermat-like functionals.

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MS60

Eikonal Functions and Their Use in Lens Design

The notion of eikonal functions goes back to Hamilton's original papers on geometrical optics. They are used by lens designers since the late 19th century mostly for notation purposes. This seems surprising since an eikonal function carries all the geometrical information on the optical element. The difficulty in using such a function in a design process is that it is a function of 4 variables which is hard to characterize or to compute. I shall present a design method that is based on eikonal functions.

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MS61

Comprehensive High-accuracy Modelling of Electromagnetic Effects in Complete Nanoscale RF Blocks

IC design automation tools are indispensable for RF designers in the transition to the nano-scale era. These tools are needed to develop nano-scale designs of unprecedented complexity and performance and, in addition, enable the achievement of single-pass design success to avoid costly re-spins and the loss of market opportunities. Next generation designs will be challenged by an increased number of trouble spots, many of which negligible at lower frequencies but representing a significant limitation for future designs. These trouble spots will have to be accounted for during the design phase in order to avoid costly mishaps that can originate potential failures and additional design and silicon iterations, and must be addressed in future design automation tools. The key to the avoidance of these trouble spots is the recognition that devices can no longer be treated in isolation. Complete RF blocks must be considered as one entity. Today, it is not possible to perform such analyses of complete RF blocks. In this presentation, we discuss methodologies to make this possible, thereby enabling designer to minimize turnaround time without compromising design quality and first-time-right requirements. An important ingredient is the benchmarking of simulations against measurements; several examples will be given.

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MS61

Nanometer-scale Integrated Circuit Thermal Analysis

Thermal analysis has long been essential for designing reliable, high-performance, cost-effective integrated circuits. The move to nanoscale fabrication processes is increasing the importance of quantum thermal phenomena. Accurate thermal analysis of nanoscale ICs containing hundreds of millions of devices is challenging. In this talk, I present ThermalScope, a multi-scale thermal analysis method for nanoscale IC design. It unifies microscopic and macroscopic thermal physics modeling methods. It supports adaptive multi-resolution modeling. Together, these ideas enable efficient and accurate characterization of nanoscale quantum heat transport as well as chip–package level heat flow. ThermalScope is designed for full-chip thermal analysis of billion-transistor nanoscale IC designs, with accuracy at the scale of individual devices.

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MS61

Using an Open Source PDE Solver to Model Deposition Processes

Deposition processes such as electrochemical deposition or chemical vapor deposition are best represented mathematically by a system of partial differential equations (PDEs) that govern the bulk transport as well as boundary conditions that govern the motion of the interface onto which material is deposited. In order to derive and solve these equations, techniques such as the level set method or phase field method are required. These are generally hard to program and require specialized knowledge and sophisticated numerical methods that are not readily available to most interested parties. This presentation will describe an open source PDE solver (FiPy http://www.ctcms.nist.gov/fipy) that can be used to easily pose and solve equations that arise from models of deposition processes. A number of examples will be demonstrated including models of superconformal electrodeposition, diffusion-limited leveling and the electrochemical phase field model. The presentation will also emphasize the improvements that are still necessary to make FiPy more accessible to a wider user base and the need for more community participation in order to drive these improvements.

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MS61

A Novel Method for Nano-scale VLSI Circuit Performance Verification with Parameter Variations

Abstract unavailable at time of publication.

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MS62

Existence and Stability of Counter-propagating "Nearly-two-soliton" Solutions in the Fermi-Pasta-Ulam Lattice

We study the interaction of small amplitude, long wavelength solitary waves in the Fermi-Pasta-Ulam model with general nearest-neighbor interaction potential. We establish global-in-time existence and stability of counter-propagating solitary wave solutions. These solutions are close to the linear superposition of two solitary waves for large positive and negative values of time; for intemediate values of time these solutions describe the interaction of two counter-propagating pulses. These solutions are stable with respect to perturbations in ℓ^2 and asymptotically stable with respect to perturbations which decay exponentially at spatial $\pm\infty$.

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MS62

Frequency Analysis of Surface Water Waves

I will speak on the wave motion on the interface between the vacuum and the two-dimensional fluid under the influence of gravity and surface tension. I will begin by a precise account of the formulation of the surface water-wave problem and of its linearization. I will give the frequency analysis of the linearized problem in the presence of surface tension and discuss its implication on stability. This work is joint with Hans Christianson and Gigliola Staffilani.

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MS62

Instability of Solitary Water Waves

Consider 2D irrotational solitary water waves without surface tension. The highest wave has a 120 degree angle at the crest, known by Stokes in 1880. In a recent paper (IMRN, 2008), I proved linear instability of solitary waves which are higher than the wave of maximal energy and lower than the wave of maximal travel speed. It is also shown that there exists unstable solitary waves approaching the highest wave. The instability of these large solitary waves are related to the breaking of water waves.

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MS62

Stability of Solitary Waves on Water

The talk will discuss most recent development on the stability of two- and three-dimensional solitary waves on the surface of water with finite depth using various model equations or exact Euler equations. It was known that these equations have solitary-wave solutions and the stability of these waves in many problems is still open. Here, various stability results for these waves will be addressed, such as transverse stability, spectral stability or conditional stability.

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MS63

Treecode Algorithms for the Helmholtz Equation

Fully Lagrangian frameworks have long been one of the primary tools in the kinetic simulation of plasmas. The Vlassov-Poisson/Vlassov- Maxwell system is cast as a collection of charged particles, which are evolved under the action of self consistent long range fields. Boundary Integral Treecode (BIT) is a method for computing the long range forces in $O(N \log N)$ operations. The underlying idea is to efficiently compute particle-cluster interactions using recurrence relations. We are working towards solving the Darwin approximation of these electro-magnetic simulations using a treecode framework.

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MS63

A WENO Algorithm for Radiative Transfer of Photons by Hydrogen Gas in the Early Universe

The first radiation sources in the universe are expected to have coupled the Hydrogen ion spin temperature to the gas kinetic temperature via scattering in the Lyman-alpha resonance which is called the Wouthuysen-Field effect. By developing a numerical solver for the photon distribution of Hydrogen gas we give an estimation of the time scale for the onset of this coupling. This algorithm is based on the weighted essentially non-oscillatory (WENO) scheme for Boltzmann-like integrodifferential equations.

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MS63

A Discontinuous Galerkin Method for the Wigner-Fokker-Planck Equation

The Wigner-Fokker-Planck (WFP) equation governs the evolution of an open quantum system, coupled to its environment. It is a kinetic model used to model a range of quantum systems and devices. Recent analytic progress has increased demand for numerical approaches to the WFP equation. I will present a Discontinuous Galerkin scheme for the WFP equation with a general potential. It is adaptable, and may use polynomial and non-polynomial approximation spaces.

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MS63

Numerical Simulations of Multi-phase Complex Fluids

We model the multi-phase systems of the complex fluids by a diffuse-interface energetic approach which involves a nonlinear system for the flow velocity field, labeling variable and liquid crystal director field which came from the Ericksen-Leslie theory. An efficient and accurate numerical scheme is proposed and implemented for the coupled nonlinear system in 2d and 3d domain. Furthermore, we use this phase field framework to model and simulate the mixture between the liquid crystal polymer droplet and another viscous isotropic fluids of Landau-de Gennes theory.

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MS64

High Order Integral Equation Methods for Diffraction Problems on Open Surfaces

We present a set of fully regularized, weighted, second kind integral equations which provide a generalization of the Calderon formulae for diffraction problems on open surfaces. Further, we derive spectral quadrature rules for those equations, which, in conjunction with the use of Krylov-subspace iteration linear methods, lead to very accurate and fast solutions in two and three dimensions. We provide various illustrations on non-trivial geometries, such as arrays of disc, resonant cavities and chains of Moebius Strips.

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MS64

Application of BEM in Photoacoustic Spectroscopy

Quartz-enhanced photoacoustic spectroscopy is a new technique for the detection and quantification of trace gases. The method is based on the conversion of optical radiation to an acoustic pressure wave, which is then detected by a quartz tuning fork resonator. A key component of a computational model for such sensors involves solving a forced time-harmonic acoustic wave equation in an unbounded domain. We solve this equation using the Boundary Element Method.

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MS64

Discretization and Fast Solution of Parabolic Boundary Integral Equations

Boundary integral formulations for parabolic problems have the form of weakly singular Volterra equations. We discretize time with a singularity corrected trapezoidal rule and space with a standard quadrature rule for surface integrals of smooth functions. The complexity of the direct evaluation of the discretized operator grows quadratically in the number of space and time nodes. We discuss a fast method with almost linear complexity and conclude with applications to solidification and melting problems.

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MS64

Boundary Element Methods for Maxwell's Equations

We consider the boundary element method to solve problems of electromagnetic scattering. The talk focuses on two different representation formulas for the solution.

- We deduce a new representation of the double layer potential in terms of well known potentials (Helmholtz equation). Not only in what concerns the numerical realization, but also for theoretical studies, this is advantageous.
- We have a closer look at the low frequency problem and find a new formulation that should cope with this problem.

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MS65

Multiple Time Scale Methods for Delay Differential Equations: Experiments, Simulations, and Asymptotics

The response of a nonlinear optical oscillator subject to a delayed feedback is described by an integro-delay differential equation exhibiting three distinct time scales. Using multiple scale asymptotic techniques, we find two distinct routes to self-pulsing. Of particular interest is the onset of fast bursting oscillations on the top of a slowly-varying periodic solution that we describe by a slowly varying map coupled to a differential equation. Theoretical and experimental observations are in excellent agreement.

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MS65

Asymptotic Methods in Finance

Abstract unavailable at time of publication.

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MS65

Asymptotic Analysis of Narrow Escape Problems for Diffusion in Microdomains

A common scenario in cellular signal transduction is that a diffusing surface-bound molecule must arrive at a localized signaling region on the cell membrane before the signaling cascade can be completed. In order to determine the time-scale for this process, we calculate asymptotic results for the mean first passage time for a diffusing particle confined to the surface of a sphere in the presence of multiple partially absorbing traps of small radii. In addition, asymptotic results for the related narrow escape problem of calculating the mean first passage time for a diffusing particle inside a sphere with small traps on an otherwise reflecting boundary are also given. The asymptotic analysis relies on detailed properties of certain Green's functions related to the sphere. The asymptotic results are shown to compare favorably with full numerical results.

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MS65

Perturbation Analysis for Impulsive Differential Equations

Models for dynamical systems that include short-time or abrupt forcing can be written as impulsive differential equations. Applications include mechanical systems with impacts and models for electro-chemical spiking signals in neurons. We consider a model for spiking in neurons given by a nonlinear ordinary differential equation that includes a Dirac delta function. Ambiguities in how to interpret such equations can be resolved via perturbation methods and asymptotic analysis of delta sequences.

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MS66

Pulses and Dynamics in Mode-locked Lasers

Mode-locked lasers can generate ultra-short optical pulses, with durations ranging from hundreds of picoseconds down to a few femtoseconds. An important mathematical model includes the so-called master laser equation. Recently a distributed modification of this system, the so-called power-energy saturation (PES) equation has been The PES model admits mode-locked localized pulse solutions as well as soliton bound states under wide ranges of the parameters for both constant dispersion as well as dispersion-managed systems in both the anomalous and normal regimes. Localized modes are found by mode-finding methods and direct numerical simulation indicates that they evolve from general initial data.

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MS66

The Dispersion-managed Ginzburg-Landau Equation and its Applications to Femtosecond Lasers

Many kinds of femtosecond lasers produce pulses that undergo significant changes in the cavity during each roundtrip. I first introduce the dispersion-managed Ginzburg-Landau equation (DMGLE) as a model for the long-term dynamics of systems with large variations of dispersion, nonlinearity and gain in a general setting. I then explain how the DMGLE models femtosecond lasers, and I characterize its solutions. For moderate gain/loss variations, solutions of the DMGLE are approximated by those of the dispersion-managed nonlinear Schroedinger equation (DMNLSE), the effect of gain/loss dynamics being to select one solution in the one-parameter family of solutions of the DMNLSE.

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MS66

Using the Nonlinear Schroedinger Equation for Precision Optical Measurements

Frequency combs produce light that is both broadband and highly coherent. However, their operation relies on the nonlinear Schroedinger equation, in particular to achieve the broad spectral output. Because it is a highly nonlinear system, this comb output can exhibit noise due to small changes in the input conditions. We will discuss some of the high-resolution measurements possible with frequency combs as well as some of the limitations posed by noise on the comb sources.

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MS66

Intensity Dynamics in a Waveguide Array Laser

We consider numerically the optical field dynamics of a five-emitter laser array subject to a linearly decreasing injection current. Among the observed behaviors is a robust oscillatory power output with a nearly constant π phase shift between the oscillations of neighboring waveguides. In this regime, the frequency of oscillation increases with injection current, and higher harmonics are produced. Additionally, experimental results from a five-emitter AlGaAs quantum dot laser array and theoretical predictions are in agreement.

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MS67

Axisymmetric Stokes Flow Past Orthogonally Intersecting Spheres

An axisymmetric Stokes flow past a rigid body of two orthogonally intersecting spheres in a uniform flow along the line of centers is considered and a method of solution is discussed for this problem. The method is also applied to the rigid body when the flow is perpendicular to the line of centers and the corresponding solution is discussed.

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MS67

General Solutions for Singular Fluctuations, Resonant Disturbances, and Hidden Perturbations of

the Couette Flow

General solutions of the Navier-Stokes equations of the Couette flow in the class of the one-center spatial Boussinesq-Rayleigh-Taylor series, the one-center temporal Boussinesq-Rayleigh-Taylor series, and the two-center spatiotemporal Taylor series are compared. Instability of the Couette flow and generation of deterministic chaos in the Couette flow by singular fluctuations, resonant disturbances, and hidden perturbations are considered.

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MS67

A New Method of Resolution of Multi-scale Hydrodynamic Clusters of Zeroes and Extrema

An algorithm of numerical resolution of multi-scale clusters of zeroes and extrema of the Couette flow is discussed as a successful alternative to conventional methods, robustness of which is limited by mono-scale zeroes. The algorithm is based on multi-scale nested meshes, through which the algorithm effectively finds potential clusters and, like a digital microscope, recurrently zooms into nested scales of the clusters until their resolution. Several examples of implementation of the search algorithm are presented.

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MS67

An Interesting Application of a General Solution of Stokes Equations

An arbitrary Stokes flow of a viscous, incompressible fluid past a sphere with a thin coating of a fluid of a different viscosity is considered and a general method is suggested for this problem by applying a recent solution of Stokes equations. The flow quantities like drag and torque experienced by the fluid coated sphere are discussed and some interesting observations are made about the conditions under which the drag reduces.

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MS68

A Special Decomposition of Planar Graphs with Large Girth

Abstract unavailable at time of publication.

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MS68

Generalized Balloons and the Chinese Postman Problem in Regular Graphs

We previously determined the minimum size of a maximum matching in a connected $(2r+1)$-regular graph with n vertices; the extremal graphs have cut-edges. In this paper, we prove a lower bound for the minimum size of a maximum matching in a t-edge-connected r-regular graph with n vertices, for $t \geq 2$ and $r \geq 4$. The bound is sharp infinitely often and improves a recent result of Henning and Yeo. We also study the Chinese Postman Problem, the problem of find a shortest closed walk traversing all edges. In a cubic graph, this is equivalent to finding a smallest spanning subgraph in which all vertices have odd degree. We establish an upper bound in terms of the number of vertices. The bound is sharp infinitely often, achieved by the connected cubic graphs having the smallest maximum matchings.

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MS68

Vertex, Edge, and Vertex-edge Random Graphs

We consider three classes of random graphs: edge random graphs, vertex random graphs, and vertex-edge random graphs. Edge random graphs are Erdős-Rényi random graphs, vertex random graphs are generalizations of geometric random graphs, and vertex-edge random graphs generalize both. The names of these three types of random graphs describe where the randomness in the models lies: in the edges, in the vertices, or in both. We show that vertex-edge random graphs, ostensibly the most general of the three models, can be approximated arbitrarily closely by vertex random graphs, but that the two categories are distinct.

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MS68

Acquisition Parameters in Graphs

Let G be a graph with weight 1 on each vertex. When a vertex u has a neighbor v whose weight is at least that on u, an *acquisition move* transfers all weight from u to v. The *acquisition number* of G, written $a(G)$ and introduced by Lampert and Slater in 1995, is the minimum number of vertices with positive weight after a sequence of acquisition moves. We introduce two variations. *Partial acquisition moves* transfer unit amounts of weight, and *continuous acquisition moves* transfer arbitrary positive amounts. The *partial* and *continuous acquisition numbers* $a_p(G)$ and $a_c(G)$, respectively, are the minimum number of vertices with positive weight after a sequence of moves in these models. We explore these three parameters, proving that they are equal on paths and cycles while differing greatly

on other families of graphs.

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MS69

Parallel Implicit Solvers in Multiphase Flow and Reactive Transport in Porous Media

We describe our experiences with implicit solvers in PFLOTRAN, a code for simulating coupled thermal-hydrologic-chemical processes in variably saturated, non-isothermal, porous media. Timestepping typically employs two sequentially-coupled implicit solves, one for multiphase fluid flow and heat transfer, and one for reactive chemical transport. We will discuss our experiences using a variety of solvers for problems drawn from real-world field sites on large-scale computing platforms such as the Cray XT5 and the IBM BlueGene/P.

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MS69

Progress on the Development of an Implicit Fully-coupled Stabilized FE Resistive MHD Solver

Fluid models of resistive MHD are multiphysics PDE systems that are strongly coupled, highly nonlinear and characterized by multiple physical phenomena spanning a very large range of length and time scales. This talk overviews progress on developing fully-coupled Newton-Krylov solvers that enable efficient fully-implicit time integration and direct-to-steady-state, continuation, and bifurcation solution algorithms. In this context the robustness, efficiency, and the parallel and algorithmic scaling of an algebraic fully-coupled multilevel preconditioner will be discussed.

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MS69

Software Development of Composite Solvers for Electrical Power Systems

The solution and analysis of multiphysics, multiscale models presents one of the major hurdles for modern applied and computational mathematics. Motivated by various applications, e.g., coupling between flow and reaction variables in groundwater modeling and coupling between core and edge models in fusion simulations, we are developing capabilities in PETSc library to ease the implementation of multiphysics simulations. Our approach includes (1) simple user specification of multimodels, (2) abstractions for managing the composition of solvers, and (3) flexible solver options and efficient solution for coupled multimodels. In this talk we present our latest progress and demonstrate our approach through a three phase instantaneous time domain simulation of electric power systems.

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MS69

Towards Fully-Implicit Parallel Adaptive Solution of Mantle Convection Problems

Mantle convection is the principal control on the thermal and geological evolution of the Earth. A basic model consists of an advection-diffusion equation coupled to a non-linear Stokes equation. We are developing *Rhea*, a new generation mantle convection code incorporating parallel adaptive mesh algorithms to enable simulations that can resolve features down to 1 km on a global scale. We discuss *Rhea*'s parallel scalability and limitations of our current semi-implicit solver. To overcome restrictions we examine design and implementation of a fully-implicit solver. We conclude with a discussion of the importance of fully-implicit solvers for adjoint-based inverse solution.

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MS70

The Calderon Problem and EIT for Low Regularity Conductivities

Abstract unavailable at time of publication.

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MS70

Mathematical Problems Arising in the Diagnosis and Treatment of Breast Cancer

Abstract unavailable at time of publication.

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MS70

Reconstructing Small Perturbations of an Interface from Modal Measurements

Abstract unavailable at time of publication.

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MS70

Regularization of a D-bar Method for Electrical Impedance Tomography

Abstract unavailable at time of publication.

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MS71

Multi-Model Approaches to Simulating Metabolic Networks: A Chlamy Case Study

Metabolic networks can be modeled dynamically (e.g., mass action kinetics) and with respect to non-equilibrium steady states (e.g., Energy Balance Analysis). The use of one approach to inform and, in some cases, simplify the other holds the promise of a more robust overall model for genome-scale networks. We present a case study in which the behavior of the photosynthetic apparatus of S-deprived C. reinhardtii is investigated, and discuss computational challenges of increasing system size.

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MS71

Parallel Computing and Model Representation for Metabolic Simulation: Issues for in Silico Whole Cell Models

The ability both to understand what a biochemical model actually represents, to simulate accurately the underlying mechanism, and to find and use such models for reexamination and extension, depends on precise meaning in the model representation. We will discuss our efforts on the construction of central carbon metabolism, energy metabolism, and hydrogen-producing pathways in the green alga, Chlamydomonas reinhardtii, including the workflow of our Python-based toolset for Systems Biology Markup Language model merging and conversion. We will also discuss opportunities for high-performance metabolic simulation, and how open-source tools are being used in our High-Performance Systems Biology Toolkit, a C/C++-based package for metabolic model parameter sampling and optimization.

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MS71

High Performance Systems Biology Tools

As metabolic models grow, all phases of the modeling workflow, from model editing, to simulation, to parameter identification, to model optimization, become intractable with current tools. In this talk we will describe the mathematical and computer science aspects of our effort in the NREL Scientific Computing Group to build a suite of high performance parallel tools enabling the creation, exploration, and optimization of whole-cell metabolic models.

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MS71

Computational Analysis of Cardiac Energetics in Failing Hearts

The failing heart is hypothesized to suffer from energy starvation. Using a computational model of cardiac energetics, we analyzed data from a canine left ventricular hypertrophy model to determine how the energy state evolves due to changes in key metabolic pools. Our findings-confirmed by in vivo 31P-MRS-indicate that the transition between the clinically observed early compensatory phase and heart failure and the critical point where the transition occurs are emergent properties of cardiac energy metabolism.

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MS72

Deforming Composite Grids for Multi-Physics Modeling

The description of physical systems by mathematical models often divides a domain naturally into regions where different physical processes are taking place. Multi-fluid problems and fluid-structure interaction are common examples of such systems. In this talk we discuss new developments for treating multi-material and multi-fluid problems. The approach taken here uses interface fitted composite grids which deform to conform to the boundary between regions. The efficacy of this approach is judged through application to two-material problems and comparison to existing techniques.

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MS72

Improved Localization Conditions for the Multiscale Finite Volume Method: An Iterative Approach

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

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MS72

High-Order Constrained Transport Methods for Ideal MHD

Constrained transport (CT) methods were introduced by Evans and Hawley (1988) as an extension of the Yee scheme (1966) to ideal magnetohydrodynamics (MHD). In their standard form, CT methods are typically either second or fourth order accurate, since they are based on central differencing. In this talk we will present an arbitrary-order CT method that is based on a mixed finite element/finite difference formulation. The proposed method is applied to several standard ideal MHD test cases.

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MS72

Title unavailable at time of publication

Abstract unavailable at time of publication.

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MS73

The Effects of Stimulated Raman Scattering on Pulse Propagation in Massive Multichannel Fiber Optics Communication Systems

Stimulated Raman scattering is one of the most important processes affecting pulse propagation in massive multichannel optical fiber telecommunication systems. It induces energy exchange in pulse collisions, which is independent of the frequency difference between the channels, and thus poses a challenge for modeling. In this work we develop a mean-field model for the propagation - a stochastic nonlinear Schrödinger equation, which takes into account changes in pulse amplitude and frequency as well as emission of continuous radiation. Our analysis and numerical simulations show that the normalized moments of pulse parameters grow exponentially with propagation distance. Furthermore, the dynamics leads to relatively high values of the bit-error-rate (BER) and the main contribution to the BER is caused by large position shifts induced by relatively large amplitude values.

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MS73

Impact of Random Variations on Ultra-short Solitons in Cubic Nonlinear Media

Using recently developed techniques to coarse-grain noise in multi-scale systems, I derive a stochastic version of the short-pulse equation (SPE) from Maxwell's equations. With this stochastic short-pulse equation at hand, I will discuss the impact of noise on ultra-short Sakovich solitons.

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MS73

Bifurcation of Bisoliton Solutions in Optical Fiber Links with Dispersion Management

Solitons in fiber optical systems with dispersion management have been studied intensively and put to use by the communication industry. In fall of 2005, experimental group in University of Rostock, Germany, showed that bound pairs of dispersion managed solitons may form a bound state, bisoli- ton, and propagate in such a way over long distances. In the limit of strong dispersion map NLSE is reduced to an integral equation. The naive iteration procedure for solving the integral equation is shown to be unstable. A method to stabilize the iterations is developed. Using this method we have found parametric bifurcation of bisolitonic solutions.

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MS73

Instanton Analysis of Low-density Parity-check Codes in the Error-floor Regime

Standard iterative decoding of a graph based code does not guarantee convergence. For some codes decoded iteratively, as for the model [155,64,20] code considered, cycling of iterations is observed for lower weight configuration of the noise dominating the error floor asymptotic. The behavior of the iterative decoding near this special configuration is chaotic. As shown in [Stepanov, Chertkov'06] the iterative scheme can be improved to enforce the iteration convergence. We discuss in this talk how the decoding improvement affects the dangerous cycling configuration.

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MS74

Duality Between Stochastic Dominance Con-

straints and Risk Measures

We consider stochastic optimization problems with second order nonlinear stochastic dominance constraints formulated as a relation of Lorenz curves. The relation can be characterized in terms of rank dependent utility functions, which generalize Yaari's utility functions. We establish two duality relations. First, we prove that Lagrange multipliers associated with these constraints can be identified with rank dependent utility functions. Furthermore, we demonstrate that mean-risk models with law invariant coherent risk measures appear as dual optimization problems to the problems with stochastic dominance constraints as well.

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MS74

A Branch-and-Cut Algorithm without Binary Variables for Optimization with First-Order Dominance Constraints

We present a branch-and-cut algorithm for solving stochastic programs with first-order stochastic dominance (FSD) constraints. The algorithm enforces the non-convex FSD constraint through branching, and hence requires no binary variables. This enables the use of an existing cutting plane method for solving the second-order dominance relaxation to yield bounds. The key challenge we address is how to adapt this relaxation to the constraints imposed by branching.

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MS74

Sample Average Approximation of Linear Stochastic Dominance Constrained Programs

We propose a Sample Average Approximation (SAA) method for the optimization problems with multi-dimensional linear second-order stochastic dominance constraints. The approach is shown to converge exponentially fast as the sample size increases. We present a cut generation algorithm to solve the resulting problem. Statistical lower and upper bound computing procedures are given for the optimal objective value.

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MS74

Risk-Averse Dynamic Programming

We shall discuss stochastic dynamic optimization problems, in which preferences are modeled by dynamic measures of risk. We shall develop the theory of conditional measures of risk to derive dynamic programming equations for such problems. We shall also discuss methods for solving these equations.

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MS75

High Performance Community Detection in Networks

We will discuss the state of the art in methods for detecting communities in networks, especially in the context of high-performance computing (HPC). Modularity maximization has an associated resolution limit, but we will discuss tolerating that limit. We will also abstract recent literature in community detection via machine learning, and its HPC challenges. We will conclude with some recent algorithms of ours for finding communities of various sizes without tuning a coarseness parameter.

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MS75

Challenges in Combinatorial Scientific Computing

Computation on large combinatorial structures has become fundamental in many areas of data analysis and scientific modeling. However, the field of high-performance combinatorial computing is still in its infancy, at least as compared to numerical supercomputing. I will describe several challenges for combinatorial scientific computing in algorithms, tools, architectures, and mathematics. I will draw examples from several applications, and will highlight our group's work on algebraic primitives for computation on large graphs.

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MS75

Discovering Molecules of Interest by Combinatorial*Computational*Chemoinformatics (C-cube) Approach

The developed combinatorial*computational*chemoinformatics (C-cube) approach uses the power of computers to combinatorially generate chemical species different by structure and/or composition, calculate their properties and perform screening to identify novel molecules/materials of desired properties. The massive amounts of data are analyzed to understand the structure-property relations. The latter may be used to perform further navigated searches in chemical space, where only molecules that are likely to exhibit the property of interest are fully characterized.

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MS75

Software Tools for Large Scale Combinatorial Computing

Combinatorial computing is now being increasingly used by a wide variety of practitioners to gain insight into the structure of their problems. Combinatorial methods are being applied in fields as diverse as ecology, biology, finance and social networking. We believe that a lack of easy to use software tools is preventing wider use of combinatorial techniques. Matlab made numerical computing accessible to a number of scientists, and today is widely used for numerical computing. Star-P takes this one step further, making parallel computing accessible to users of the Matlab programming language. Augmenting Matlab's array based programming language and Star-P's parallel constructs with capabilities for combinatorial computing can result in a powerful platform for numerical and combinatorial computing.

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MS76

Steric Hindrance Effects on Surface Reactions

Many biological and industrial processes have reactions which occur in thin zones of densely packed receptors, which can be modeled as a reacting surface. Interpreting biosensor data correctly is difficult since large ligand molecules can block multiple receptor sites, thus skewing the kinetics. General mathematical principles are presented for handling this phenomenon, and a surface reaction model is presented explicitly. In the limit of small Damkohler number, the non-local nature of the system becomes evident in the association problem, while other experiments can be modelled using local techniques. Explicit and asymptotic solutions are constructed for large-molecule cases motivated by experimental design.

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MS76

Continuum Models of Chemical Reaction Networks

Deterministic models of chemical reaction networks often consist of systems of coupled ODE. We introduce a technique by which reaction systems exhibiting repetitive structure may be approximated by reduced numbers of PDE. The method is similar to approximating a chain of springs as an elastic continuum. We will discuss the method in general and, for a particular reaction system, show that, in an asymptotic sense, the qualitative behavior of the original ODE system is preserved.

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MS76

Exhaustion of Nucleation in a Closed System

The classical ideas of aggregation kinetics traditionally model the initial nucleation of supercritical clusters (Zeldovich) and the final late stage coarsening (Lipshitz and Sleozov). A complete history, including the intermediate stages, is generally believed to be outside the reach of classical modeling. But in the limit of small initial oversaturation, there is a separation of time and cluster size scales that leads to an asymptotic analysis of the whole aggregation process, based solely on the founding ideas. The characteristic times to "exhaust" the initial nucleation and to achieve the self similar coarsening are for the first time identified in terms of physical parameters and the initial oversaturation.

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MS76

Mathematical Models of Electro- and Magneto-Capillary Interactions

Capillary surfaces have long been of physical and mathematical interest. Today, their study is more relevant than ever, with interest sparked by applications such as self-assembly, bio-mimetic devices, microelectromechanical systems, and bio-mechanics. Such systems become even more complicated and interesting when electric or magnetic fields are introduced. In this talk, we explore recent experimental and theoretical work in this area.

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MS77

Stability Analysis of the Mode-Locking Dynamics in a Laser Cavity with a Passive Polarizer

A low-dimensional model is constructed via a variational formulation to describe the mode-locking dynamics in a laser cavity with a passive polarizer and dissipative effects. It is shown that the mode-locked state is completely characterized by the fixed point of the reduced system. The transient oscillations period and decay rate to this fixed point is calculated via a center-manifold reduction and shown to depend upon the net cavity gain and the gain bandwidth.

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MS77

Spatio-temporal Dynamics in Mode-locked Lasers

Spatial effects are incorporated into the master mode-locking equation. The role of spatio-temporal effects in the pulse dynamics and is studied using asymptotic and numerical methods.

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MS77

Interference of Quantum Trajectories in High Harmonic Generation

We present experimental observations of quantum paths in below-threshold high-harmonic generations. In addition to answering fundamental questions pertaining to the extremely nonlinear high harmonic process, these studies will allow one to control the amplitude to phase-noise conversion in high harmonic generation more precisely. Understanding these noise processes will be crucial for future experiments on precision spectroscopy and high-resolution quantum control utilizing XUV frequency combs.

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MS77

Computational Modeling of a Similariton Fiber Laser

The recent development of similariton fiber lasers has enabled the generation of high power femto-second pulses and high repetition rate frequency combs. We describe a computational model of an experimental similariton laser incorporating a highly nonlinear fiber amplifier. We use this model to the determine the shape of the pulses and to compute the evolution of the timing jitter. We compare the results to those obtained from a generalized perturbation theory that we have developed.

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MS78

Electrodiffusion Modeling and the Retina

Electrodiffusion models and numerical methods for their solution will be discussed for simulating ion propagation and electrical transmission in and between nerve cells of the retina. Robust numerical methods (especially TRBDF2) needed to solve these stiff nonlinear differential equation models – which include advection-diffusion, Poisson's equation, and ODEs for modeling ensembles of channels – will be emphasized.

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MS78

Electrodiffusion of Charged Hard-Sphere Ions Through Biological Ion Channels: Theory Predicts Experiments

Biological ion channels are proteins that form a pore to conduct ions like Na^+, K^+, and Ca^{2+} across membranes down electrochemical potential gradients. Calcium channels conduct Ca^{2+} preferentially to the monovalent cations even though Ca^{2+} is at 100+ times lower concentration. Electrodiffusion of these ions (described as charged, hard spheres using density functional theory of fluids) reproduces and predicts experiments for the ryanodine receptor calcium channel. The balance of ion size and electrostatics determines selectivity.

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MS78

Fully Continuum Modeling of Electro-diffusion-reaction Processes in Realistic Biomolecular Systems

The Poisson-Nernst-Planck equation is used to model fully-continuum diffusion-reaction processes within biological systems, and appears to be a framework to study even more general molecular solvation effects. We'll discuss our recent developments in PNP methodologies, including the finite element solution, mesh generation, regularization of the Poisson-Boltzmann equation, and some PNP model extensions. The work is applied to both simple model systems and a biological event in the synapse: the consumption of the neurotransmitter by the enzyme acetylcholinesterase.

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MS78

A Three-Dimensional Model of Cellular Electrical Activity

We present a three-dimensional model of cellular electrical activity. This model takes into account the three-dimensional geometry of biological tissue as well as ionic concentration dynamics, both of which are neglected in conventional models of electrophysiology. We use both asymptotic and analytic methods to study the system of equations. We find in particular that the model possesses multiple temporal and spatial scales. This has important consequences for the development of an efficient numerical scheme. This modeling methodology is applied to cardiac physiology. Numerical simulations with this model is used to explore the characteristics of a recently observed anomalous mode of cardiac action potential propagation: cardiac propagation without gap junctions.

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MS79

Unavoidable Subhypergraphs Beyond the EKR Bound

Let $\mathbf{a} = (a_1, a_2, \ldots, a_p)$ be a sequence of positive integers, its sum is k. The system of k-element sets $\{F_0, F_1, \ldots, F_p\}$ is called an $\mathbf{a}$-*cluster* if
— their union has $2k$ elements,
— $|F_i \setminus F_0| = a_i$ (consequently these sets are disjoint outside F_0), and
— every element of F_0 belongs to exactly p of these sets (i.e., the sets $F_0 \setminus F_i$ form a partition of F_0). Suppose that $\mathcal{F}$ is a k-uniform hypergraph on n vertices, $|\mathcal{F}| > \binom{n-1}{k-1}$ and n is sufficiently large (with respect to k), and suppose that $\mathbf{a} \neq (1, \ldots, 1)$. We **conjecture** that $\mathcal{F}$ must contain an $\mathbf{a}$-cluster. We prove the case when all $a_i \geq 2$ with $\max a_i > 2$.
The case $p = 1$ corresponds to the Erdős-Ko-Rado theorem, in the case $p = k$ (i.e, $a_1 = \ldots = a_k = 1$) the threshold (in general) is slightly larger, it is $\binom{n}{k-1}$.
This is a strengthening of earlier results by Katona, Frankl and Füredi, and most recently by Mubayi, Keevash and Ramadurai. Most of the new results presented are joint with L. Özkahya.

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MS79

Combinatorial and Probabilistic Aspects of Simplicial Complexes

A simplicial complex X is a finite family of sets that is closed under inclusion. Namely, if A is a member of X and B is a subset of A then B is a member of X as well. If the largest set in X has cardinality d+1, then X is said to have dimension d. Clearly a one-dimensional simplicial complex is nothing but a graph. On the other hand a simplicial complex is also a way of describing geometric objects and have an important role in topology. Simplicial complexes have been used in the past to solve several important problems in combinatorics and in theoretical computer science. In this talk I report about several recent papers where we seek to investigate simplicial complexes from the perspective of modern combinatorics. The probabilistic method plays an important role and in particular one of our main objectives is to develop a higher-dimensional analogue of the Erdos-Renyi G(n,p) model of random graphs. Many many fascinating open questions suggest themselves. The new results are from joint papers with Meshulam, Rosenthal and Aronshtam.

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MS79

Catalan Structures

If n men and n women sit at a circular table, in how many ways can they be divided into n male-female pairs so that no pair's direct line of conversation (i.e. line of sight) rudely crosses that of another pair? For example, if all of the men sit in a row on one half of the table and all the women on the other, there's only one non-crossing pairing. On the other hand, if no two people of the same sex sit adjacently, the number of non-crossing pairings is the nth Catalan number. Expressing the number of pairings as a nice function of some straightforward parameters of the seating arrangement appears to be difficult. However, we do have nice results for seating arrangements in which any run of men (i.e. a maximal group of adjacently seated men) is always followed by a run of the same number of women. Interestingly, the problem comes from random matrix theory. We also found connections to several things including the enumeration of certain types of dissections of polygons. Amdeberhan and Stanley independently investigated closely related problems.

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MS79

Counting Increasing Sequences that Lie Below a Given One

Abstract unavailable at time of publication.

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MS80

Implicit Nonlinear Solvers in Coupled Core-Edge Fusion Models

Modeling of the plasma core and edge relies on the use of implicit solvers. Both regions require implicit solvers because of diffusive transport with the fluxes being highly nonlinear functions of the plasma parameters. Additionally the edge requires implicitness to deal with short timescales, while the resulting solution is smooth and slow. FACETS (Framework Application for Core-Edge Transport Simulations) is coupling these two implicitly solved systems. Solutions will be presented.

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MS80

Preconditioned Jacobian Free Newton-Krylov Methods for Reactor Fuel Performance Simulation

The simulation of nuclear reactor fuel performance involves complex thermomechanical processes between fuel pellets, made of fissile material, and the protective cladding barrier that surrounds the pellets. This talk develops a three dimensional thermomechanical and oxygen diffusion equation system that is solved in a parallel, fully-coupled, fully-implicit manner using a preconditioned Jacobian-free Newton Krylov method. Both steady state and transient results are examined to compare the outcome with the literature. INLs BISON fuels performance code is used to perform this analysis.

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MS80

Algorithms and Software for Multiphysics Compu-

tational Nuclear Engineering

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

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MS80

A Multiscale Preconditioner for Nonlinear Multiphysics Problems in Porous Media

The mortar mixed finite element method can be viewed as a multiscale method, with recent developments showing that the construction of a multiscale basis can greatly reduce the computational cost. We show that this multiscale basis does not need to be recomputed if used as a preconditioner for a Krylov method. We apply this preconditioner to a nonlinear multiphysics problem in porous media.

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MS81

Time-Periodic Interfacial Fluid Flows

We introduce a numerical method for computing time-periodic solutions of nonlinear partial differential equations. As an application of this method, we study time-periodic solutions of the Benjamin-Ono equation. We find a large number of such solutions. In particular, we find continua of genuinely time-periodic solutions connecting different traveling waves. This investigation leads us to exact, explicit formulas for these solutions. We will also discuss applications of this method to computing time-periodic vortex sheets and water waves. This is joint work with Jon Wilkening.

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MS81

Title unavailable at time of publication

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MS81

Infinite-energy Statistical Solutions to the Equations of Incompressible Fluids in the Plane

We construct statistical solutions to the Navier-Stokes equations in the whole plane by making a limiting argument involving a sequence of solutions to the Navier-Stokes equations on balls of increasing radii. Such solutions encompass initial velocities having bounded vorticity, which includes the important special case of vortex patch initial data. We then construct an infinite-energy statistical solution to the Euler equations by making a vanishing viscosity argument.

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MS81

Recent Results for the Vortex-wave System

The vortex-wave system is the coupling of the 2D vorticity equation, for the evolution of a continuous distribution of vorticity, with the point-vortex system. This terminology was introduced by Marchioro and Pulvirenti in 1991. They also proved existence and uniqueness of solutions when the initial data is a vortex patch with point vortices outside the patch, a result recently generalized by Lacave and Miot. Our main result is existence of a suitably defined weak solution for vorticity in L^p, $p > 2$.

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MS82

Computational Aspects of the Multidimensional Moment-constrained Maximum Entropy Problem

Recently the author developed a numerical method for the multidimensional moment-constrained maximum entropy problem, which is capable of solving maximum entropy problems in the two-dimensional domain with moment constraints of order up to 8, in the three-dimensional domain with moment constraints of order up to 6, and in the four-dimensional domain with moment constraints of order up to 4. Here we present an exposition of the current methods and results of this work.

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MS82

Enforcing Positivity in Spherical Harmonic Moment Closures

We present recent results using variational techniques to develop positive, spherical harmonics-based approximations to the neutral particle transport equation. One approach uses filtered expansions to give positive solutions and reduce wave effects in the solutions. The other approach solves a local optimization problem to produce a reconstruction of the kinetic density that is positive and close to the original spherical harmonics reconstruction. We compare solutions using our filtered expansions and local optimization method to the standard spherical harmonics expansions, Monte Carlo, diffusion, discrete ordinates, and analytic transport solutions.

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MS82

Convex Duality and Entropy-based Moment Closures: Characterizing Degenerate Densities

Entropy-based closure seeks to determine, given finitely many moments (macroscopic densities), the distribution function that minimizes the kinetic entropy subject to satisfying the moment constraints. Unfortunately, in many situations, macroscopic densities can take on values for which the constrained minimization problem has no solution. In this paper, we give a geometric description of these so-called degenerate densities in a general setting. This result is important for further assessment and implementation of entropy-based moment closures.

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MS82

Moment Equations in Kinetic Theory: An Overview and Outlook

This talk will introduce the use of moment closures as approximation technique in kinetic theory. We will review the framework given by kinetic theory in particular that of gases. Moment equations replace the stochastic description by deterministic partial differential equations. They will be discussed from a mathematical, physical and numerical point of view. A major focus will are recent developments, for example in entropy maximizing closures, regularization techniques and numerical methods.

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MS83

Numerical Valuation of Commodity American Options in the Non-Markovian Approach by the Semilinear Evolution Equation and Multi-Layered Tree Methods

We present the numerical valuation of American options on commodity spots, forwards and swaps in the non-Markovian approach introduced earlier by the author. The numerical valuation is based on the semilinear evolution equation for American options and the multi-layered tree methods both introduced earlier by the author. We compare the computational efficiency of these methods and apply them to modeling the NYMEX American options on crude oil and natural gas in the non-Markovian approach.

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MS83

A Regime Switching Model for the Term Structure of Credit Risk Spreads

We consider a rating-based model for the term structure of credit risk spreads such that the credit-worthiness of the issuer follows as a discrete state space Markov chain. This approach entails a progressive drift in credit quality towards default, as opposed to a single jump to bankruptcy as in so-called hazard-rate models. Rating-based models are particularly useful for pricing securities whose payoffs depend on the rating of the issuer. Our approach is a SDE formulation of the Martingale approach by Jarrow, Lando, and Turnbull (1997).

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MS83

A Numerical Analysis of American Options with Regime Switching

A finite element method and a simple lattice method are proposed for numerical valuation of American options under a regime switching model. Numerical results are presented to compare our methods and to examine their accuracy for various combinations of parameters. The dependency of early exercise prices and option prices on parameters are also investigated numerically.

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MS83

An Inverse Problem Arising from the Black-Scholes

Model

In this talk we consider an inverse problem of determination of volatility for the option pricing model. We assume that the volatility depends on both time and underline financial asset. By giving option price of a financial asset, the volatility can be determined. Some numerical results will also be discussed.

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MS84
Anti-Cycles in Directed Graphs

An anti-cycle is an orientation of an undirected even cycle C such that every vertex has either in-degree zero or out-degree zero. In this talk we give minimum degree and neighborhood union conditions which guarantee that a digraph D contains a hamiltonian anti-cycle. In addition, we give a minimum degree condition which guarantees that a digraph D contains anti-cycles of all possible lengths, and some generalizations.

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MS84
Path Spectrum Sets

A path in a graph is maximal if it is not a proper subpath of any other path of the graph. The *Path Spectrum* of a graph is the set of lengths of all maximal paths in the graph. A set of positive integers is an *Absolute Path Spectrum* if there are an infinite number of graphs with that Path Spectrum. A summary of results on the path spectrum for graphs will be presented along with some new results on Non-Path Spectrum Sets, on Absolute Path Spectrum Sets, and the Path Spectrum of trees.

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MS84
Cycle Spectra of Hamiltonian Graphs

The cycle spectrum of a graph G is the set of lengths of cycles in G. Let $s(G)$ denote the size of the cycle spectrum of G. Jacobson and Lehel asked for lower bounds on $s(G)$ when G is a 3-regular Hamiltonian graph on n vertices. We show that if G is a Hamiltonian graph on n vertices with m edges, then $s(G)$ is at least $\sqrt{(4/7)(m-n)}-1$. When n is even, the complete bipartite graph $K_{n/2,n/2}$ provides an example where $s(G)$ is at most $\sqrt{m-n}+1$. Nevertheless, we conjecture that when G is Hamiltonian and 3-regular, $s(G)$ is at least cn for some constant c.

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MS84
A Survey of Results on Graph Linkage

For a given graph H, a graph G is H-linked if G has an H-subdivision no matter how the branch set is given. This notion of H-linkage generalizes a lot of well-studied ideas such as graph connectivity, k-orderability and k-linkage. Since it was formly introduced in 2005, this notion has attracted quite a bit of attention. In this talk, we will give a brief survey of known results about H-linked graphs.

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MS85
Hierarchical Regularization for Edge-preserving Reconstruction of PET Images

PET data consists of counts of photons originating from random events, resulting in data-noise that is well-modeled by a Poisson distribution. Since the associated Poisson regression problem is ill-posed, regularization is required. Following the Bayesian paradigm, we introduce a hierarchical regularization model that allows for the formation of edges in reconstructed images. A numerically effective algorithm for solving the associated minimization problem is presented. We test our methodology with both simulated and real data PET data.

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MS85
Regularization Parameter Selection Methods for Ill-Posed Poisson Regression Problems

In image processing applications, image intensity is often measured via the counting of incident photons. When the associated Poisson maximum likelihood estimation problem is ill-posed, however, regularization is needed. Regularized Poisson maximum likelihood estimation has been extensively studied by the authors, however, the essential problem of choosing the regularization parameter remains unaddressed. In this talk, we present three statistically motivated methods for choosing the regularization parameter.

Numerical examples will be presented to test the methods.

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MS85

A Preconditioned LSQR Approach to a Structured Least Squares Problem in Adaptive Optics

A Kronecker-product structured, rank-deficient, least-squares problem from adaptive optics is presented. By using statistical properties of known data sets, an all-purpose preconditioner can be computed once and stored, utilizing the generalized singular value decomposition. For a given data set, a Tikhonov-type regularized solution can be obtained in just a few iterations of preconditioned LSQR with an appropriate regularization parameter, which is chosen based on statistical properties of the noise.

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MS85

Numerical Methods for Bayesian Experimental Design

Experimental design is an important topic in physical and biological and engineering applications. While the topic has been studied at depth for over-determined well-posed problems, it has been hardly addressed for rank deficient ill-posed problems. In this talk we examine the A and E Bayesian optimal designs. In particular, we examine efficient methods for large scale design of inverse problems.

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MS86

Heat Diffusion and the Leidenfrost Effect

A mathematical model is developed for the Leidenfrost effect on an axisymmetric droplet. The shape of the droplet will be considered first and best fit formulae are presented relating the droplet surface area to volume. The full model for Leidenfrost will then be discussed. The effect may be described by three first order ordinary differential equations involving the volume, evaporation rate and vapour film thickness. Numerical and experimental results will then be compared.

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MS86

Simulating the Cooling of a Cheese Cylinder Floating in Brine

A mathematical model for the temperature of a cylindrical cheese product floating in a channel of brine is presented. The cross section of the cylinder is that of a circle truncated by a chord. The equilibrium positions and the stability of these positions in the brine are discussed. Due to the unusual model geometry and the non-homogonous boundary conditions, a finite volume, numerical solution for the temperature is provided.

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MS86

Mathematical Modeling of Heat and Mass Transfer Processes in the Drying of Spherical Particles in Fluidized Beds

The drying of spherical particles in a fluidized bed is considered. This process is of great interest in the food and pharmaceutical industries as the final structure of many products is determined by the drying process and this final structure will significantly influence their end-use properties. During the drying process, moving interfaces (e.g., between wet and dry zones) develop inside the particle, separating the product into regions that have quite disparate structures with an attendant diversity of thermo-physical and mechanical properties. Accurate modelling of the locations of these interfaces and the transport phenomena that take place there is challenging but essential if the model is to correctly predict the final attributes of the product. Mathematically, one has a Stefan problem defined by a pair of parabolic partial differential equations with a free boundary and appropriate boundary conditions; these relate the temperature and moisture content within the product. A new finite difference method for solving this problem is presented and its convergence properties are studied. A special approach to error analysis is necessary to justify the accuracy of this method. The efficiency of the method is also of interest since it will be used in the future to model polydispersed materials.

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MS86

A Degenerate Singularly Perturbed Parabolic Problem Modelling Heat Transfer

The problem $\varepsilon u_{xx}(x,t) - x^{\alpha}u_t(x,t) = f(x,t)$ is considered on the domain $(0,1)\times(0,T]$, with Dirichlet initial-boundary conditions. Here ε is a small positive parameter and α is a positive constant. The presence of a small diffusion coefficient and the degeneracy of the coefficient of u_t along $x=0$ combine to introduce certain difficulties into the problem, which is not easily solved using standard numerical techniques. Under suitable hypotheses on f, a decomposition of the solution u and bounds on its derivatives are obtained. These bounds are used to analyze a finite difference method on a modified Shishkin mesh. Nonlinear analogues of this problem arise in the modelling of temperature distributions in certain chemical engineering applications. Consider also the transfer of heat in a medium moving with velocity x^{α} and conducting heat only across the flow along the t axis (e.g., for a viscous liquid between plates which are moving at different velocities, one has $\alpha = 1$).

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MS87

Nonlinear Waveguide Arrays as an Ultrafast Saturable Absorber

Ultrashort pulses are coupled to an AlGaAs waveguide array. Frequency-resolved optical gating (FROG) measurements show the pulses at the output of the central waveguide in the array have a set spectral phase independent of the input spectral phase. Time domain electric fields retrieved from the FROG measurement corroborate this observation, and the phenomenon is shown to be power dependent.

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MS87

A SVD-based Method for Determining Large Deformations in Optical Systems

In optical systems the events of interest, i.e., ones that cause errors, are large pulse deformations. We present a method to determine such large deformations by exploiting the mathematical structure of the governing equations and the singular value decomposition to formulate a constrained optimization problem. These results then guide importance-sampled Monte-Carlo simulations to determine the events' probabilities. The method works for a general class of intensity-based optical detectors and for arbitrarily shaped pulses.

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MS87

Modeling Laser Mode-locking for Generation of Multiple Pulses per Cavity Round-trip

Abstract unavailable at time of publication.

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MS87

Phase Noise and Rare Events in Mode-locked Lasers

In recent years there has been much interest in predicting errors in nonlinear optical systems such as optical fiber communication systems and femtosecond lasers. Using semi-analytic and numerical methods, one can directly reconstruct probability distribution functions (pdfs) of signal parameters whose large deviations (rare events) are responsible for errors. For some applications of interest – specifically lasers – we are specifically interested in errors due to phase noise.

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MS88

Subsonic Propagation of an Interfacial Crack with a Finite Friction Zone Ahead

A 2d-problem on a semi-infinite crack with a friction zone ahead propagating along a rigid/elastic interface is solved by quadratures. In the sub-Rayleigh and super-Rayleigh regimes, the problem is equivalent to a vector Riemann-Hilbert problem with a piece-wise constant matrix coefficient with three points of discontinuity. The matrix coefficient is factorized in terms of hypergeometric functions. A transcendental equation for the friction zone length is derived.

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MS88

Trapped Modes and Slow Sound in Elastic Waveguides

Trapped modes are non-trivial localised eigensolutions that can exist within guiding structures due to perturbations in guide thickness, localised inhomogeneity or curvature. Trapped modes are well-known within acoustic, or their equivalent quantum, guides where they are called bound states. This talk will cover their occurrence in elastic guides where it can be shown that group velocity plays a key role. Recently there has been interest in so-called slow sound/ light in elastic/ optical waveguides, by considering periodic stripped waveguides and Bloch waves one can demonstrate that there are quasi-periodic trapped modes and that these correspond to the observed slow modes. The existence of these modes is demonstrated both numerically and using an asymptotic approach based upon perturbing about the cut-off frequencies of the guide.

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MS88

Bending Instabilities of Biological Soft Tissues

The severe bending of a thick block leads to the apparition of wrinkles on its inner curved face. Incremental nonlinear elasticity predicts that this buckling occurs when line elements contract by 44% for neo-Hookean solids. We consider the incorporation of strain-stiffening effects into the constitutive model. For models used for biological soft tissues such as arteries and veins, we find that wrinkles appear at much more moderate amounts of bending than for the neo-Hookean solid.

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MS88

Elastic Wave Scattering from a Cavity in a Pre-Stressed, Nonlinear Elastic Medium

We study the canonical problem of scattering from an isolated cavity situated in a nonlinear elastic material which has been pre-stressed via some hydrostatic pressure imposed in the far field. The pre-stress induces non-homogeneous stress and stretch distributions around the cavity and therefore the problem requires careful analysis in order to determine how a subsequent small-amplitude incident plane-wave is scattered. Low frequency, horizontal shear wave scattering is studied and by using matched asymptotics, we show how the leading order scattered field (monopole and dipole terms) is modified by the nonlinear pre-stress.

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MS89

On the Mathematical Role of Entropy Variables in Numerical Methods for Boltzmann Moment Closure

Entropy variables appear prominently as Lagrange multipliers in Levermore's Boltzmann moment closure theory [C.D. Levermore, "Moment Closure Hierarchies for Kinetic Theories", J. Stat. Phys., Vol 83,1996]. These same variables play an essential role in the analysis of finite element methods for system of conservation laws with convex entropy extension. In the present talk, a brief outline of this theory is given for the discontinuous Galerkin discretization of Boltzmann moment systems with Levermore closure [T. Barth, "On Discontinuous Galerkin Approximations of Boltzmann Moment Systems with Levermore Closure", CMAME, Vol 195, 2006]. The main theoretical results from this analysis are sufficient conditions to be imposed on the numerical flux function so that system energy/entropy stability is obtained. A class of energy/entropy stable numerical fluxes are also explicitly given in this previous work. More recently, a new numerical flux function has been developed that also satisfies these technical conditions while performing significantly better in actual computations. In the remainder of the talk, we discuss a general software platform developed for Boltzmann moment closure research and current work addressing the well-known degeneracy problem associated with Levermore's exponential conjugate entropies as identified in [M. Junk, "Domain of Definition of Levermore's Five Moment Systems", J. Stat. Phys, Vol. 93, 1998] and further elucidated recently in [C.D. Hauck et. al, "Convex Duality and Entropy-Based Moment Closures: Characterizing Degenerate Densities", CNLS Report, Los Alamos National Laboratory, 2007].

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MS89

Discrete Galerkin Methods with Entropy Variables and Explicit Time Integrators: A Numerical Study with the Shallow Water Equations

We investigate discrete Galerkin methods for conservation laws that use entropy variables to generate entropy-stable schemes. Unfortunately, the fully discrete scheme is also fully implicit, often making it prohibitively expensive. For shallow water equations, we investigate schemes that use explicit time integrators and solve convex optimization problems to find local expansion coefficients. Such schemes fit squarely into the emerging paradigm of data-parallel computing, since the optimization algorithm can be managed by local processing units.

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MS89

On the Gaussian Closure in Fluid Regimes

Various moment closures have been proposed to reduce classical kinetic equations in transition regimes. Perhaps the simplest of these is the Gaussian (ten moment) closure with a diffusive correction. We show how this closure yields a moment system with an entropy structure that captures most known fluid dynamical regimes. This include some regimes that are not captured by the compressible Navier-Stokes system, such as the "ghost effect" regime studied by Sone. We also show how the system recovers certain "beyond Navier-Stokes" terms in the Chapman-Enskog expansion.

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MS89

Non-linear Closures for the Linearized Boltzmann Transport Equation

We have developed a new parametric non-linear closure for the 1-D slab-geometry Sn equations with linear-discontinuous (LD) spatial differencing that is strictly positive and yields the set-to-zero fixup equations in the limit as the parameter is increased without bound. We present results indicating that for an appropriate range of parameteric values, our new method is strictly positive, efficient, and yields solutions that rapidly approach the standard LD solution as the spatial mesh is refined.

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MS90

New Results on Linear Formulations of Directed Minimum Cut and GTSP

We present new mathematical programming approaches to solving a classic variant of the Traveling Salesman Problem (GTSP) using integer programming. One of the challenges in modeling GTSP is to achieve as small a linear programming formulation as possible of minimum directed cut, or equivalently, minimum spanning tree. We describe our progress in this endeavour.

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MS90

Exploring Relaxations of Max Cut

We study integer programming formulations and semidefinite and linear relaxations of the maximum cut problem. We describe an approach to matching and improving on the semidefinite relaxation that uses linear programming technology and exploits the special structure of the maximum cut problem. We also offer alternative methods of solving the semidefinite relaxation.

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MS90

A New Linear Formulation for Minimum Cut and Relaxation for TSP

Existing linear formulations for minimum cut require at least n*m variables and constraints for a graph with n vertices and m edges. These formulations parallel early algorithmic approaches to finding globally minimum cuts using flows. We present the first formulation to beat this bound, one that use $O(n^2)$ variables and $O(n^3)$ constraints. Our formulation implies a smaller compact linear relaxation for the Traveling Salesman Problem that is equivalent in strength to the standard subtour relaxation.

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MS90

Fractional Decomposition Trees: A (Parallel)

Heuristic for Integer Programs

We present a parallelizable algorithm for finding a feasible solution for a integer program. The algorithm runs in time polynomial in the input size and is guaranteed to find a feasible integer solution for any problem class that has a finite integrality gap. The algorithm is based on convex decomposition of scaled linear-programming relaxations, so in general it provides a suite of integer solutions. A faster heuristic gives only one feasible solution.

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MS91

A Front-Fixing Finite Element Method for the Valuation of American Put Options on Zero-Coupon Bonds

A front-fixing finite element method is developed for the valuation of American put options on zero-coupon bonds under a class of one-factor models of short interest rates. Numerical results are presented to examine our method and to compare it with the usual finite element method. A conjecture concerning the behavior of the early exercise boundary near the option expiration date is proposed according to the numerical results.

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MS91

Pricing American Options under a Stochastic Volatility Model with Jumps

A linear complementarity problem (LCP) is formulated for the price of an American option under the Bates model. The underlying partial integro-differential operator is discretized using a finite difference method and a simple quadrature. Time stepping is performed using a componentwise splitting method. It leads to the solution of sequence of one-dimensional LCPs which can be solved very efficiently using the Brennan and Schwartz algorithm. Numerical experiments demonstrate the componentwise splitting method to be fast and accurate.

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MS91

Superconvergence Estimates of Finite Element Methods for American Options

In this talk we are concerned with finite element approximations to the evaluation of American options. Firstly, following W. Allegretto etc, SIAM J. Numer. Anal. 39 (2001), 834–857, we introduce a novel practical approach to the discussed problem, which involves the exact reformulation of the original problem and the implementation of the numerical solution over a very small region, such that this algorithm is very rapid and highly accurate. Secondly, by means of a superapproximation and interpolation post-processing analysis technique, here we present the sharp L^2 and L^∞ norm error estimates and the H^1-norm superconvergent estimate, respectively, for this finite element method. As a by-product, the global superconvergence result can be used to generate an efficient a posteriori error estimator. Finally, several numerical examples are presented to demonstrate the theoretical results.

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MS92

Strong Hamiltonian Properties in 4-connected Graphs

A well known conjecture of Matthews and Sumner is that every 4-connected $K_{1,3}$ graph is hamiltonian. In this talk we look at pairs of forbidden subgraphs of the form $\{K_{1,3}, H\}$ that imply a 4-connected graph is pancyclic. The particular graphs H are all generalized nets, that is, a triangle with an end vertex of a path identifed at each vertex of the triangle. The net $N(i, j, k)$ denotes the triangle with paths of lengths i, j and k rooted at the three vertices. We consider the situation where $i + j + k = 5$. These pairs are extensions of the forbidden pairs characterizing the 3-connected pancyclic graphs.

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MS92

A Generalization of Kundu's k-Factor Theorem

Given nonnegative integer lists $d_1, d_2, \ldots, d_j$, the degree sequence packing problem is to determine if there exist edge-disjoint graphs $G_1, G_2, \ldots, G_j$ on the same vertex set such that G_i has degree sequence d_i. A famous example of a result on degree sequence packing is Kundu's k-factor theorem, which states that if d is a graphic sequence, and if the sequence d' obtained by adding k to each entry of d is also graphic, then there exists a graph G with degree sequence d and an edge-disjoint k-regular graph on the same vertex set. We will consider extensions to Kundu's theroem, particularly when a graphic sequence can be packed with multiple 1-regular graphs.

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MS92

Forbidden Subgraphs and 2-Factors

For a set $\mathcal{H}$ of connected graphs, a graph G is said to be $\mathcal{H}$-free if G does not contain any member of $\mathcal{H}$ as an induced subgraph. In this talk, we investigate the sets $\mathcal{H}$ such that every $\mathcal{H}$-free graph, possibly except for a finite number of exceptions, has a 2-factor. More formally, let $\mathcal{G}$ be the set of all the finite connected graphs of minimum degree at least two, and define $\mathcal{G}(\mathcal{H}) = \{G \in \mathcal{G} : G \text{ is } \mathcal{H}\text{-free}\}$ and $\mathcal{F} = \{G \in \mathcal{G} : G \text{ has a 2-factor}\}$. We consider $\mathcal{H}$ such that $\mathcal{G}(\mathcal{H})$ is an infinite set while $\mathcal{G}(\mathcal{H}) - \mathcal{F}$ is a finite set.

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MS93

Modeling the Early Dynamics of Rodent Malaria Infections

What determines the dynamics of asexual parasites in blood during acute primary malaria infections, and why do some strains of malaria reach higher peak parasite densities than others? We use mathematical models to explore the effects of parasite growth rate, RBC limitation and innate and adaptive immunity on the dynamics of rodent malaria infections.

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MS93

In-host Dynamics of Mixed Malaria Infection with Adaptive Immunity

Multiple pathogen species or strains interact within host environment by competing for available resources, and by stimulating cross-reactive immune responses. Such "competition" plays important role for understanding the dynamics of infections, both on individual and community levels. It allows among other to study such evolutionary adaptations, as drug resistance or virulence. We shall outline some basic principles and mathematical approaches to modeling host-parasite interactions with adaptive immunity, to be applied to study in-host competition of multi-strain malaria pathogens, and its effect on evolution of virulence.

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MS93

The Dynamics of Mosquito Populations

A deterministic differential equation model for the population dynamics of mosquitoes studied. Conditions for the existence and stability of a non-zero steady state vector population density are derived. These reveal the existence of a threshold parameter, the vectorial basic reproduction number, and instability via a Hopf Bifurcation to periodic solutions. Asymptotic perturbations are used in analysis. Results capture the possibility of studying the population dynamics of mosquitoes without recourse to external seasonal forcing.

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MS93

A Mathematical Model of the Within – Vector Dynamics of the Plasmodium Falciparum Protozoan Parasite

Based upon experimental data, a mathematical model is developed that simulates the within-vector dynamics of Plasmodium falciparum in an Anopheles mosquito. The model takes as input a mosquito blood meal and the final output is the salivary gland sporozoite load, a probable measure of mosquito infectivity. Sensitivity analysis of the model parameters suggests that reduction of gametocyte density in the blood meal most significantly lowers mosquito infectivity, and is thus an attractive target for malaria control. The model is used to investigate the implication of incomplete fertilization on optimal gametocyte sex ratio. Model extensions and other model implications for malaria control are also discussed.

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MS94

Morozov's Discrepancy Principle and Tikhonov-type Functionals

This talk deals with regularization theory for linear and ill-posed inverse problems in Hilbert spaces. We focus on Tikhonov functionals

$$\Gamma_{\alpha,\delta}(x) = \|Ax - y^\delta\|^2 + \alpha\Omega(x),$$

where the classical L_2-penalty term is substituted by a more general functional Ω. We show under which conditions the minimization of such functionals, combined with Morozov's discrepancy principle as a parameter choice rule for the regularization parameter α, forms a regularization method. Further we show convergence rates.

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MS94

Regularization Parameter Selection for Total Variation

The selection of optimal regularization parameter plays an important role in the correct implementation of Total Variation (TV) regularization. The Unbiased Predictive Risk Estimator (UPRE) has been shown to give a very good estimate of this parameter for Tikhonov Regularization. In this talk we propose an approach to extend the UPRE method to the TV problem by utilizing the idea of linearization and randomization, which provides a good estimation.

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MS94

Regularization with Diagonal Weighting Matrices

The numerical linear algebra community typically uses regularization methods to solve ill-posed problems, while statistical approaches involve specifying a priori information about the parameters. The chi-squared method developed by the authors and colleagues combines the best solution methodologies from both communities by finding solutions that do not assume specific probability distributions, and use matrices to weight the regularization term. We will describe an efficient algorithm for the determination of these weighting matrices, and show results.

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MS94

Statistical Properties of Tikhonov Regularization for Least Squares Problems: Relationships between Unbiased Predictive Risk and χ^2 Methods for Parameter Estimates

Unbiased predictive risk successfully estimates the regularization parameter for Tikhonov least squares functionals, given information on statistical properties of measurements errors. But effective implementation for large scale problems is hindered by the need to estimate the trace of the influence matrix. In contrast, the χ^2 regularization parameter estimator can be implemented efficiently. Here we discuss the relationship between the two methods, as illustrated by their similar performance on some test problems and for image restoration.

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MS95

The Double Majorization Order

The double-majorization order is a partial order extending the classical majorization (=dominance) order on partitions. We will discuss some of its properties. This is joint work with Allison Cuttler and Mark Skandera.

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MS95

Families of Subsets with Forbidden Subposets

We consider the problem of determining the maximum size $\mathrm{La(n,H)}$ of a family $\mathcal{F}$ of subsets of the set $\{1, 2, \ldots, n\}$, subject to the condition that a certain subposet is excluded. For instance, Sperner's Theorem solves the problem for H being a two-element chain P_2, giving $\mathrm{La(n, P_2)} = \binom{\mathrm{n}}{\lfloor \frac{\mathrm{n}}{2} \rfloor}$. We survey results of this kind, an area promoted in recent years by Gyula O. H. Katona, including our newest bounds on $\mathrm{La(n,H)}/\binom{\mathrm{n}}{\lfloor \frac{\mathrm{n}}{2} \rfloor}$ when H is the four-element diamond poset B_2 (joint with Linyuan Lincoln Lu).

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MS95

Random Erdős-Ko-Rado

Let $3 \le k < n/2$. We prove the analogue of the Erdős-Ko-Rado theorem for the random k-uniform hypergraph $G^k(n,p)$ for various ranges of p, k, n. Along the way, we prove that every nontrivial intersecting k-uniform hypergraph can be covered by $k^2 - k + 1$ pairs, which is sharp as evidenced by projective planes. This improves upon a result of Sanders. Several open questions remain.

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MS95
Interval Partitions and Stanley Depth

In this paper, we answer a question posed by Herzog, Vladoiu, and Zheng. Their motivation involves a 1982 conjecture of Richard Stanley concerning what is now called the Stanley depth of a module. The question of Herzog et al., concerns partitions of the non-empty subsets of $\{1, 2, \ldots, n\}$ into intervals. Specifically, given a positive integer n, they asked whether there exists a partition of the non-empty subsets of $\{1, 2, \ldots, n\}$ into intervals, so that $|B| \geq n/2$ for each interval $[A, B]$ in . We answer this question in the affirmative by first embedding it in a stronger result. We then provide two alternative proofs of this second result. The two proofs use entirely different methods and yield non-isomorphic partitions. As a consequence, we establish that the Stanley depth of the ideal $(x_1, \ldots, x_n) \subseteq K[x_1, \ldots, x_n]$ (K a field) is $\lceil n/2 \rceil$.

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MS96
Speakers To Be Announced

To Be Announced.

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MS97
Speakers To Be Announced

To Be Announced.

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MS98
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PP0
A Stochastic Approach to Modeling Acid Precipitations Impact on a Tri- trophic Aquatic Ecosystem

We implemented an empirically-based Markov Chain to model variable environmental conditions of an acidified lake. Simulations were run to represent a given time frame of varying conditions that may impact ecosystem dynamics. The simulation results were then compared with a deterministic approach using optimal environmental conditions as well as the mean environmental conditions from the stochastic model. Advisor: Peter Kramer, Rensselaer Polytechnic Institute

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PP0
AWM - Optimal Control of Species Augmentation Using a Continuous Time Model

Species augmentation is a method of reducing species loss via augmenting declining/threatened populations with individuals from captive-bred or stable, wild populations. We developed a differential equations model and optimal control formulation for continuous time augmentation of a general declining population. We found a characterization for the optimal control and show numerical results for scenarios of different illustrative parameter sets. This work is a first step toward building a general population augmentation theory which accounts for complexities inherent in many conservation biology applications.

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PP0
AWM- Minimal Swimmer Models Using the Method of Regularized Stokeslets

The Method of images for regularized Stokeslets is applied to minimal swimmer models representing micro-organisms. Resistance matrices are used to compute the efficiency of a representative Spirochete in the presence of a surface. The effect of the gap thickness on the efficiency is elucidated. Further extending the method to the minimal swimmer model consisting of a cell body and flagellar bundle, we take advantage of the methods ability to incorporate the interactions between the cell body and the flagellar bundle and comparably predict experimental characteristics specific to E.Coli. We have further demonstrated the versatility of the method to predict behavior of other micro-organisms that possess similar structure, by showing the dependence of the swimming speed on the geometric parameters such as the amplitude of the helical structure and the number of pitches and gap thickness. The effect of interactions between the cell and bundle on the forward swimming speed is elucidated numerically.

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PP0

Agent Based Model of Spread of Disease Coupled with Fear

Traditional epidemiological models of the spread of diseases consist of a system of differential equations. These models assume uniform mixing of the population. This project uses agent based modeling to remove this assumption. In addition, the model allows fear to infect the agents. This induces the agents to either flee their neighborhood or remove themselves from the network altogether for a period of time. The resultant dynamics can generate waves of infection that the ordinary differential equation system can not produce. Advisor: Dana Fine, University of Massachusetts-Dartmouth

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PP0

Micro-Mirror Method for Catadioptric Sensor Design

Many applications such as surveillance, photography, and robot navigation, require wide-angle imaging with minimal distortion. We propose a method to design visual sensors for any application, using a mirror, a micro-mirror array, and a camera. We discuss the system of PDEs whose numerical solutions give the mirror surface and the micro-mirror array distribution. We give an example of our novel method; a sensor that annihilates blind spot in automobiles.

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PP0

AWM - Simulation of Multiphysics and Multiphase Flow

First , we develop high order Discontinuous Galerkin methods for three-phase flow arising in mixing of oil, gas and water in porous media. We solve sequentially the equations for oil pressure, water saturation and gas saturation on fully unstructured grids Second, we analyze the coupling of Navier-Stokes and Darcy equations which models groundwater contamination through lakes and rivers. We obtain optimal convergence of two numerical schemes based on classical and discontinuous finite element methods.

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PP0

Effective Mass Density of a Periodic Array of Acoustic Media

Effective mass densities of periodic microstructures have been posed in different forms for waves propagating in solid-in-fluid composite materials. In this study, we develop a homogenization analysis to derive a unified formula of effective mass density for acoustic solid embedded in fluid. It is shown that the effective mass density is modified from the harmonic mean of the composing mass densities according to the detailed microstructure in respective physical dimensions. Some earlier results of effective mass density derived by other authors are recovered under simplified assumptions, whence we may assess their validity and limitations. The anisotropy of effective mass density with respect to the direction of wave propagation is also discussed.

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PP0

Extensional Flow of a Wormlike Micellar Mixture

We consider the inhomogeneous extensional response of a new consti- tutive model, the VCM model, that has been developed to describe con- centrated solutions of wormlike micelles. The time dependent numerical analysis is carried out in a slender filament formulation appropriate for elongational flows of complex fluids. The simulations show that elongat- ing filaments described by the VCM model exhibit a dramatic and sudden rupture event similar to what is observed in filament stretching experiments of wormlike micelles. This work was partially supported by NSF #DMS-0807395

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PP0

AWM - A Score Based Combinatorial Approach to Detecting

Modern genetic epidemiology is an interdisciplinary subject, which heavily rely on quantitative (mathematical and statistical) models and tools to find out the relationships between disease traits and the underlying genetic characteristics. To detect gene-gene interactions, we proposed a new method which is an important modification and extension of the current popular Multifactor- Dimensionality

Reduction (MDR)* method. Our method can deal with family data (which is more important and informative in clinical data), and also improved computational efficiency by incorporating a likelihood score for each individual.

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PP0

AWM - Mathematically Modeling the Impact of a Population Bottleneck on the Immune Memory Repertoire

Certain viruses kill off memory T-cells early in infection and thus create lymphopenic conditions in a process called active attrition; following this, memory and nave T-cells proliferate (and differentiate if necessary) to refill the memory T-cell compartment. I mathematically examine how active attrition and subsequent lymphopenic proliferation impact the memory CD8+ T-cell repertoire using a combination of hypergeometric distributions and Markov birth processes. This gives insight into how the immune memory repertoire changes with infections.

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PP0

Path Integral Option Pricing on Nvidia Gpus

Many-core graphical processing units (GPUs) have demonstrated significant performance results for acceleration of numerical algorithms compared to general-purpose central processing units. However, applications have to be implemented for highly-parallel, multi-threaded programming models with not fully supported IEEE 754 double precision capabilities. We discuss the implementation of a path integral algorithm for pricing of American options on NVIDIA GPUs, its performance and accuracy (both in single and double precision).

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PP0

AWM- An Analytically Derived Amplitude Equation to Describe Alternans in Cardiac Tissue

An arrhythmia is any disturbance from the normal periodicity of the heart beat. Alternans is one type of arrhythmia which can be a precursor to potentially fatal conditions of the heart. In this research, I use existing models describing electrical wave propagation in the heart along with techniques of singular perturbation theory to derive and analyze an equation describing the onset and development of alternans in cardiac tissue.

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PP0

A Fast, Accurate, and Parallel Numerical Solver for Multiple Scales Problems

This ongoing undergraduate research project centers on developing differential equation solvers that are rapid and accurate for a class of multi-scale biochemical reaction problems. We developed a hybrid asymptotic numerical polyalgorithm that caters to the local structure of the solution and can be parallelized. We present results of an initial value problem for the Riccati equation with two possible local algorithms using a multi-stage piece-wise linear interpolation of the nonlinear term or a Taylor series method. Advisor: Raymond C. Y. Chin, Indiana University Purdue University Indianapolis

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PP0

Vaccinating Against HPV in Dynamical Social Network

We develop a dynamical network model to examine the relative merits of strategies for vaccinating women against the sexually transmitted Human Papillomavirus, which can induce cervical cancer. The model community is represented as a sexual network of individuals with links dynamically created and destroyed through statistical rules based on the node characteristics. Various strategies for distributing an allotted number of doses of vaccine are tested for effectiveness in reducing the incidence of cervical cancer. Advisor: Peter Kramer, Rensselaer Polytechnic Institute

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PP0

A Fundamental Solution Method for Computing Pressure and Streamlines Distributions in Reservoirs Containing Thin Barriers

Numerical simulation of flow around thin geological barriers is standard topic in reservoir simulation. In this context very refined or special designed grids are used to simulate the barriers effects, which is not a well justified effort in many reservoir problems. This article presents a new numerical method for approximating pressure and streamlines distributions in reservoirs containing thin barriers. It is based on the fundamental solution method and complex variables representations of thin barriers singularities to produce an original, efficient and simple algorithm. The new method is tested and validated on reservoirs with single, periodic, stochastically distributed barriers with multiple wells. A comparative CPU time study gives evidence that the new approach is more efficient than standard numerical finite difference method used in reservoir simulation.

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PP0

Constructing Networks for Cascade Resilience

Complex socio-economic networks need to continue functioning even if some of the nodes are compromised by a human or natural adversary, particularly where this can cause a cascade. This cascade resilience problem motivates a model under which networks are optimized for cascade resilience as well as efficiency. A topology consisting of multiple stars was shown to be highly optimal. Surprisingly, it was found that often edge density does not monotonically decrease when cascade risk increases.

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PP0

Modeling Cartilage Regeneration in the Extracellular Environment of a Cell-Seeded Hydrogel

Articular cartilage is a connective tissue lining the surface of bones in diarthrodial joints and has a limited capacity for growth and repair. Nutrient-rich hydrogels seeded with cartilage cells (chondrocytes) have potential utility as biomaterials for tissue regeneration and repair. Reaction-diffusion models of cartilage regeneration are developed for a spherical geometry that models a single cell surrounded by hydrogel. A level set method is used to model the moving interface that results from accumulation of cell-synthesized extracellular matrix as it reacts with the hydrogel.

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PP0

Immersed Finite Elements: Galerkin, Finite Volume Element and Discontinuous Galerkin Methods

This poster presents a system of immersed finite elements for solving elliptic interface problems on structured meshes instead of body-fitting meshes. We first construct an immersed bilinear finite element space and then prove its optimal approximate capability. Next we apply this space to Galerkin method, finite volume element method, and discontinuous Galerkin methods. Both numerical examples and theoretical analysis show that the numerical solutions of these methods have the optimal convergence rates.

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PP0

Multilevel Approximation of Option Prices

The price of an option is the expected value of the payoff, which is a function of Brownian motion via a stochastic differential equation for the underlying asset price. Thus, the option price is an infinite dimensional integral. Using a truncated Karhunen-Loève expansion to represent the Brownian motion and sampling with low discrepancy points makes the evaluation of this integral more efficient than using i.i.d. sampling. A multilevel (in dimension) approximation accelerates the convergence even further.

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PP0

Uniqueness and Reconstruction of Sound Speed in Thermo-Acoustic Tomography.

We present an overview of research dealing with the unique determination of the acoustic speed of a body, Ω, from thermo-acoustic data. The reconstruction of the electromagnetic absorption in Ω and a piecewise constant, radially symmetric acoustic speed from thermo-acoustic measurements is also demonstrated.

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PP0

A Mathematical Model of Necrotizing Enterocolitis

Necrotizing Enterocolitis (NEC) is a prevalent neonatal disease considered one of the greatest threats to the longterm health and survival of preterm infants. We present a mathematical model built on partial differential equations that reproduces the bodys inflammatory response to damage of the tissue layers of the gut. Using this model, we can examine the effects of various treatment methods for NEC, most notably the concept that breastfeeding drastically reduces the mortality rate. Advisor: Ivan Yotov, University of Pittsburgh

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PP0

Strong Approximation of Local Fields in Nonlinear Power Law Materials

We focus on developing a corrector theory that provides a strong approximation for local fields in Nonlinear Power Law Materials. The approximations are used to derive a lower bound that can be used to assess the singularity strength inside micro-structured materials.

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PP0

Correlation Transfer and Bifurcations in the Izhikevich Model

Previous studies have found that two essential features of neural firing – spike rate and neuron-to-neuron spike correlation from common inputs – are strongly related. These findings utilized a simple 'integrate-and-fire' model, leaving open the question of whether the previous findings can be extended to more biologically realistic models of neural firing. We address this here, for the two-dimensional, hybrid neuron model proposed by Izhikevich. First, we perform a bifurcation analysis to identify relevant parameter ranges. Advisor: Eric Shea-Brown, University of Washington

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PP0

Modeling, Analysis and Computation of Fluid Structure Interaction Models for Biological Systems

This undergraduate research paper presents mathematical models for the interaction of blood flow with the arterial wall surrounded by cerebral spinal fluid. The blood pressure on the inner arterial wall is modeled using a Fourier Series, the arterial wall is modeled using a spring-mass system and the surrounding cerebral spinal fluid is modeled via simplified Navier-Stokes equations. The coupled system of partial differential equations with appropriate boundary conditions are solved analytically using Laplace Transforms and are also investigated using computational tools. Applications of the model studied to intracranial saccular aneurysms will be presented. Advisor: Padmanabhan Seshaiyer, George Mason University

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PP0

Numerical Solutions for the Two Dimensional Poisson's Equation

Poissons equation is one of the most widely studied partial differential equations (PDEs) in applied mathematics. It is not only an important equation in electro-magnetics but also an equation of choice in testing numerical methods for PDEs. Research about finding and improving Poisson solver is never ending. Poisson solver can be found in the heart of many commercial software for the numerical solutions for PDEs. In most cases the solver has to be optimized by any means to improve the speed of calculations without sacrificing overall accuracy of the solutions. In this undergraduate research project, we want to study two-dimensional Poisson solver in regular domains. We will start with simple finite-difference methods. Both the second order centered difference and fourth order long stencil difference schemes will be explored. Advisor: Cheng Wang and Alfa Heryundono, UMASS Dartmouth

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PP0

Robustness of a-Posteriori Estimators for Multilevel Finite Element Discretizations of Elliptic-Parabolic Systems

We consider linear systems of PDEs $Lu+Au=f$ where u is a vector of unknowns, L is an elliptic or parabolic operator and A represents a monotone coupling. We derive multilevel schemes and a-posteriori estimators which are robust in the coefficients of L, A. Applications include double-diffusion and double-porosity models of flow in porous media, singularly perturbed reaction-diffusion and pseudo-parabolic systems. We present theoretical and numerical results.

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PP0

AWM - Two compartment motoneuron model to study self sustained firing after spinal cord injury

Spasticity occurs during the chronic stages after spinal cord injury (SCI). We extend previous modeling studies of the physiological changes in spinal motoneurons during the acute and chronic stages following SCI. Experimental data are used to determine the parameters of the two compartment conductance based differential equation model for SCI. Using mathematical analysis and simulation results, we study the effect of changes in kinetics and morphology on motoneuron excitability.

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PP0

Approximation of the Discontinuities of a Function by Its Classical Orthogonal Polynomial Fourier Coefficients

A modified Pronys method is considered to approximate the locations of jump discontinuities and the associated jumps of a piecewise smooth function by means of its Fourier coefficients with respect to any system of the classical orthogonal polynomials. Unlike the previously suggested method by the author, the modified method is robust, since its success is independent whether or not a location of the discontinuity coincides with a root of a classical orthogonal polynomial. In addition, the error estimate is uniform for any $[a, b] \subset (-1, 1)$.

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PP0

AWM - A Variational Approach to Recovering Coeffcients of Elliptic

The flow of groundwater in confined aquifers is commonly modeled by the parabolic partial differential equation (1).

$$q(x)\frac{\partial w}{\partial t} = -\nabla \cdot [p(x)\nabla w(x,t)] + R(x,t), \qquad (1)$$

where w denotes known piezometric head (given by height of water in observation wells relative to some reference datum), p denotes the symmetric hydraulic conductivity matrix, $q \geq 0$ denotes the storativity of the aquifer, and R denotes time-dependent recharge. Both p and q are considered to be properties of the soils and rock comprising the aquifer, and hydraulic conductivity, in particular, varies greatly within a given aquifer. Direct measurement of these values are impractical, and, given the wide variability of hydraulic conductivity, unlikely to be very accurate. Applying a finite Laplace transform with respect to time to (1), we obtain

$$-\nabla \cdot [p(x)\nabla u(x)] + \lambda q(x)u(x) = f(x), \qquad (2)$$

where p and q are as in (1), λ is the Laplace transform coefficient, u is the transformed head, and f contains the recharge information. A new variational inverse method may then be used to recover all 16 parameters for a given year, given measured head values on the boundary of the region in question. The development of recharge templates for months in the same season of different years with similar rainfall data is promising.

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Ian Knowles
Not Known
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PP0

Sudoku and Its Properties

I explore sudoku as viewed as a matrix, what peoperties it has, and how those properties are similar to Latin Squares, but also how they are unique. I look into the possibility of if given a completed 9x9 sudoku grid, and the grid's determinant and eigenvalues, can we construct the grid given its initial clues. I will also be developing a program to check to see if a grid is a valid sudoku grid. Advisor: Gary Davis, Saeja Kim and Steve Leon, UMASS Dartmouth

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PP0

AWM - Using Optimal Control to Study the Emergence of Synchrony in Networks of Coupled Oscillators

There is a great deal of interest in understanding how synchrony arises because of the prevalence with which it occurs in nature. We use optimal control theory to study the emergence of synchrony in a network of coupled oscillators as a function of the networks structure. In particular, the coupling strengths between oscillators are treated as control variables and are allowed to vary through time.

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PP0

A Network Theoretic Approach to Hyperspectral Image Classification

We present a new methodology for clustering pixels in spectral image data. The main algorithm is based on Mark Newman's Method of Maximum Modularity for community detection in networks. This provides not only a novel, accurate, and unsupervised clustering algorithm, but also supports a new approach to processing spectral data as networks and graphs. Because graphs and networks are based on local estimations of neighborhoods within the spectral data, algorithms based on these methods are said to be topological or geometric. For example, Basener et. al provide a robust method for Topologically Based Anomaly Detection (TAD). Following this nomenclature, we call our algorithm Topological Image Classification (TIC). Advisor: Anthony A. Harkin, Rochester Institute of Technology

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PP0

Developing An Open-Source Nonlinear Optimization Framework

We describe a new object-oriented open-source framework for Newton-like solvers for nonlinearly constrained optimization problems. Our framework includes a variety of step-computation techniques and a range of step-acceptance strategies. Our flexible framework allows us to tune the cost of the different step-computation, and choose from a broad range of step-acceptance strategies, including classical penalty functions, filters, and recent funnel ideas. We present preliminary numerical results.

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PP0

Microarray Gene Expression Profile in Hepatocellular Carcinoma after Surgical Resection

This study was conducted to characterize gene expression profile and create prediction model of recurrence in patients with surgically curable hepatocellular carcinoma. We used supervised statistical method to extract the gene expression profile through the cDNA microarray data and confirmed by RT-PCR. The experimental design procedures and the steps for selection of gene expression profile are presented. A prediction model is created for predicting good versus poor recurrence and recurrence curves are presented showing the prediction power.

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PP0

A Network Analysis of Roll-call Voting in the United Nations General Assembly

Having applications across physics, biology, and the social sciences, the study of networks provides a natural setting for analyzing roll call networks. In this study, networks of countries were built by quantifying similarities in countries voting on resolutions, and likewise networks of resolutions were also constructed. Analysis was performed on these unipartite projections while more sophisticated methods retain information about positive and negative correlations simultaneously and the bipartite network of resolutions and countries as a whole. Advisor: Peter J. Mucha, Carolina Center for Interdisciplinary Applied Mathematics and Mason A. Porter, University of Oxford

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PP0

AWM - Human Tear Film Dynamics on an Eye-Shaped Domain

We present recent progress in understanding the dynamics of human tear film on an eye-shaped domain. Using lubrication theory, we model the evolution of the tear film over a blink cycle. The highly nonlinear governing equation is solved on an overset grid by a method of lines coupled with finite difference in the Overture framework. Comparisons with experimental observations show qualitative agreement.

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PP0

Spatial Model of Direct Competition and a Shared Pathogen Between

There are many empirical and theoretical studies indicating that apparent competition resulting from the interaction of two species mediated by a common pathogen may cause the extinction of one of the species. However, there is little analysis of the more difficult model with both direct competition between species and a common pathogen and still less analysis for a spatial model with competition and disease. In the U.K. the red squirrel population has been drastically reduced by a combination of direct competition and a shared pathogen with the invasive grey squirrel [Rushton, et al, 2000; Tompkins, et al]. The authors in [Rushton, et al, 2000; Tompkins, et al] also indicated the possible importance of the spatial arrangement of both species and their movement between patches of habitat. We propose a multi-patch model with Lotka-Volterra competition and Susceptible-Infected disease dynamics with mass action and compare it to other models with only one or two of the mechanisms that are represented in our model. We fully examine the disease-free dynamics of the system and their global and local stability including analytic results such as computation of the basic reproduction number,R_0, and numerical results. We then find conditions for the stability of and use numerical results to show the behavior of endemic equilibria, including the case when one species is driven to extinction by another species in the presence of disease. Lastly, we extend some results to the case of n species.

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PP0

Modeling Intracranial Aneurysms

Arterial geometry, wall shear stress, and remodeling of the arterial wall by biological reconstitution are factors which may promote the rupture of aneurysms. A rigid arterial wall model of an intracranial aneurysm is studied numerically to investigate the relationship between these factors. Our model uses both idealized arterial geometries as well as geometries extracted from clinical imaging data. We examine the dependence of the rate of remodeling on wall shear stress by comparing the maximal shear stress to arterial wall thickness in patient data.

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PP0

Practical Sieve Implementation in Parallel Python

In Number Theory there are many implementations of sieves for finding prime numbers. The most well known, even to elementary students, is the Sieve of Eratosthenes. It is a very slow and impractical sieve for finding large prime numbers. A modern fast sieve is Carl Pomerance's Quadratic Sieve, invented in 1981. It is still the second fasted sieve even after 28 years. In my project I consider implementing the quadratic sieve on parallel processors to speed up the search for large prime numbers. Advisor: Saeja Kin, University of Massachusetts Dartmouth

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PP0

Performance of Algorithms for Numerical Valuation of Financial Derivatives on GPUs

Numerical valuation of financial derivatives can sometimes be performed in multiple ways (e.g., pricing of American call options via path-integral-, PDE-, tree-, and simulation-based procedures). In actual computational practice, algorithms for numerical valuation based on these different approaches can have significantly different performance "strengths and weaknesses". Focusing on algorithm performance issues that arise when computing on graphics processing units (GPUs), we compare and discuss performance of several GPU- and CPU-based algorithms for pricing American options.

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PP0

A New Stochastic Variational Pde Model for Soft Mumford Shah Segmentation and Denoising

In this poster, we present a new model for soft Mumford-Shah segmentation and denoising for mixture image patterns. We construct a functional with variable exponent which combines the TV-based and isotropic diffusion and we allow each pixel to belong to each image pattern with different probability. By taking different Gaussian means and variances on each image pattern, the segmentation can be more efficient and accurate.

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PP0

AWM - Guided Modes and Anomalous Scattering by a Periodic Lattice

We study a discrete prototype of anomalous scattering associated with the interaction of guided modes of a periodic scatterer and plane waves incident upon the scatterer. The transmission anomalies arise because of the non-robustness of a guided mode, a mode that exists at a specific frequency and wave number. The simplicity of the discrete prototype allows to make certain explicit calculations and proofs, and to examine details of important resonant phenomena of open wave guides.

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PP0

Integral Equation Methods for the Navier-Stokes Equations

An integral equation formulation for the two dimensional incompressible Navier-Stokes equations is presented. This formulation is designed for solving equations arising from temporal discretizations of the stream-function formulation. Solving these equations requires use of standard potential theory as well as modern fast algorithms such as the Fast Multipole Method. The result is a highly efficient and accurate treatment of the underlying equations. Results concerning stability, complexity and accuracy will be presented.

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PP0

A Novel Mathematical Model of Human Lactation

Lactation in human mothers is controlled by the interactions of several hormonal factors, including prolactin, which stimulates milk component synthesis, and oxytocin, which stimulates milk ejection. The details of prolactin control of milk synthesis during established lactation remain a mystery. This work analyzes alternative hypotheses concerning the effects of suckling on prolactin receptor regulation through a novel mathematical model of the cascade of interactions governing milk synthesis and ejection during established lactation. Advisor: Jonathan Rubin, University of Pittsburgh

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PP0

An Adaptive IHS Pan-sharpening Method

Pan-sharpening fuses low spatial, high spectral multispectral image with a high spatial, low spectral panchromatic image to obtain high spectral and spatial resolution image. Intensity-Hue-Saturation (IHS) is a commonly used pan-sharpening method. We do a comparative survey of different techniques and propose modification to the IHS to improve the quality of the final image. Our result prove that the adaptive IHS improves the quality of the final image. Advisor: Todd Wittman and Michael Moeller, Harvey Mudd College

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PP0

Gpu Enhanced Jump Diffusion Integrator

Jump diffusion models are of interest for a wide variety of systems from option pricing models to the evolution of particle distributions in plasma and beam-beam systems. We present a jump diffusion integrator which makes use of the power GPU processing to accelerate computation time. We compare this approach with traditional serial Monte-Carlo and finite-difference methods.

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PP0

A Normal-inverse Gaussian Random Walk Model for Wastewater in Fairhaven, Massachusetts

The ability to mathematically model wastewater flow has grown in importance as new technologies for wastewater management and utilization have emerged. The large number of factors that influence wastewater flow in Fairhaven, MA, such as precipitation, ground water levels, and behavioral phenomenon such as holidays, make it difficult to correlate wastewater with existing data. Tests for randomness such as autocorrelation and the Wald-Wolfowitz runs test suggest that the time series of daily wastewater flow can be modeled by a discrete Ornstein-Uhlenbeck process. Given the high kurtosis of a plot of the daily differences, a stochastic model of the daily fluctuations was modeled best by a normal-inverse Gaussian distribution. Advisor: Gary Davis, UMASS Dartmouth

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PP0
Resonant Scattering by an Open Waveguide: Dependence on Angle of Incidence and Geometry

We investigate anomalies in the transmission of plane waves across a periodic waveguide produced by resonant interaction with the modes of the guide. Through numerical computations and direct calculations for a discrete model, we learn how perturbations of the angle of incidence and the structure itself affect these anomalies. The discrete model gives an exact formula that matches the numerical results for the continuous problem. This work builds on that of Ptitsyna, Shipman, and Venakides. Advisor: Stephen Shipman, Louisiana State University

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PP0
AWM -Mathematical Analysis of a Double-Walled Carbon Nanotube Model

A recently developed mathematical model for a short double-walled carbon nanotube will be presented in the poster. The model is given as a system of two Timoshenko beams coupled through the Van der Waals force. Mathematically, it is a system of two coupled hyperbolic partial differential equations equipped with a four-parameter family of dynamical boundary conditions. The system has been reduced to an evolution equation with a nonselfadjoint matrix differential operator that is a dynamics generator. Asymptotic and spectral properties of this generator will be presented in the poster. We proved that it is a unbounded nonselfadjoint operator with compact resolvent, and that the set of complex eigenvalues of the dynamics generators asymptotically splits into four individual spectral branches, which is consistent with the physics of the model. The asymptotical distribution of the eigenvalues along each branch will be discussed.

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PP0
Laplace Energy of Graphs

We present preliminary results on the Laplacian energy of a graph. Complete graphs and star graphs have energy 2. Connected paths appear to have maximal normalized Laplacian energy for a given number of vertices. We compute expressions for the Laplacian energy of certain well known classes of graphs including cycles, paths and hypercubes. We discuss the observation that connected graphs seem to have minimal energy 2 - known to be true for bipartite graphs. Advisor: Gary Davis, UMASS Dartmouth

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PP0
Hydrodynamic Origin of Whale Flukeprints

A 'whale flukeprint' is a smooth patch that appears on the surface of the water behind moving cetaceans (whales, dolphins, porpoises). Interestingly, whether the origin of this phenomenon is a surfactant effect due to sloughing or a purely hydrodynamic effect is not agreed upon by marine biologists. This study investigates whether flukeprints can be formed from hydrodynamic forces. Characteristics of a flukeprint formed by a model fluke in a water tank are analyzed and robotic fluke prototypes are discussed. Hydrodynamic ring vortices are concluded to be the primary source of footprints. Advisor: Rachel Levy, Harvey Mudd College

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PP0
Mathematical Model of Network Adaptation in Physarum Polycephalum to Account for Robustness and Efficiency

Physarum polycephalum, a species of slime mold, has shown great capabilities in resource distribution, compromising between an efficient network with the shortest length, and a robust network that resists disruptions. We modeled this behavior using a modified flux model for sol through the tubes of slime mold. We compared our model results to reduced data in the literature and experimental data collected in our laboratory. Mathematical principles emulated by P. polycephalum could theoretically apply to current networking issues. Advisor: Louis Rossi, University of Delaware

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PP0
MHD Stability of Phase Transition Layers in the Interstellar Medium

We consider the scenario of a phase transition layer separating magnetized media of different densities and temperatures in a 2D plane-parallel geometry. We identify evaporation and condensation fronts, depending on whether there is net heating or cooling across the layer. We assess the behavior of both front types when subject to incompressible, corrugational perturbations, and explore the non-linear behavior using ATHENA, a Godunov scheme with nested and adaptive mesh capabilities for astrophysical MHD.

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PP0
Modeling Fluid Transport in Subcutaneous Tissue

The goal of this project is to produce a mathematical model of fluid flow in subcutaneous tissue. Two models have been developed: a compartment model that segregates the fluid into homogeneous regions, and a continuous model that describes the properties of the fluid at each point in space and time. Advisors: Richard Haskell and Rachel Levy , Harvey Mudd College

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PP0
Modeling Animal Gaits

We exhibit mathematical, electronic and physical models that generate animal gaits. One example of a mathematical generator is a network of eight coupled Van der Pol oscillators. When these oscillators are coupled together, the system produces patterns of relative phases that correspond to the different animal gaits. We show that this network can be used to produce primary gaits such as a walk, trot, pace and bound.

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PP0
Collimators Optimality Revisited

Collimators are essential tools in nuclear medicine and X and Gamma ray astronomy. I revisit the problem of optimal collimators, define a criterion of optimization based on uniform illumination of a sensor inside the collimator, derive and investigate the integral equation that determines the optimal collimator and show an exact solution for a particular case (when the equation is trivial enough to have such a solution), respectively examples of numerical solutions for other cases.

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PP0
Fuzzy Clustering for the Segmentation of Medical Images

We use fuzzy clustering to automatically segment tissue and organ regions in CT scans of abdominal cross-sections. The images are processed using PIGMAP with both raw pixel data and feature vectors. Results are fair, with good visual segmentation between tissue types. Progress is made toward differentiating between liver and spleen, and further work in image smoothing could provide useful results.

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PP0
G^k Blending of Non-symmetric Corner of Lowest Degree by Piecewise Algebraic Surface

In this paper, we present two methods of blending the corner of three coordinate planes with G^k continuity piecewise algebraic surfaces under non-symmetric conditions. The piecewise algebraic surfaces we obtained have the lowest degree under some specified conditions. First, we use the general method to obtain the G^1 continuity blending surfaces. For convex case, the algebraic necessary and sufficient condition of quadratic G^1 blending surface is $\frac{m_i+n_i-2}{m_in_i} = K$ and the geometric necessary and sufficient condition of quadratic G^1 blending surface is $\frac{m_i+n_i-2}{m_in_i} = K$, where K satisfied a specified condition. The algebraic G^1 condition of a piecewise algebraic surface means that the algebraic G^1 condition holds between any two adjacent pieces while the geometric G^1 condition of a piecewise algebraic surface means that this piecewise algebraic surface is both algebraic G^1 and no holes. For concave case, the algebraic necessary and sufficient condition of quadratic G^1 blending surface is $\frac{m_1+n_1-2}{m_1n_1} = \frac{m_2+n_2-2}{m_2n_2} = \frac{4m_3n_3-3m_3-3n_3+2}{m_3n_3}$. Opposite to the convex case, in concave case, we prove that any algebraic G^1 piecewise algebraic surface has at least one hole. By controlling the parameters in those necessary and sufficient conditions, we can easily adjust the blending domain and control the shape of blending surfaces. For $G^k(k \geq 2)$, we obtain the blending surface algebraically by generator basis method.

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PP0
Frequency Extraction of Electromagnetic Resonant

Structures Using Vorpal

We present results for an efficient frequency extraction algorithm based on the Finite Difference Time Domain (FDTD) method and a regularized SVD algorithm used for post-processing. For a spherical cavity relative errors are shown to be as low as 0.001% for the lower frequency modes using the parallel FDTD code, VORPAL. These results are comparable to Microwave Studio, HFSS, and Omega3p. We also present highly accurate validation results for realistic radiofrequency cavities.

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