CP1
Mimetic Discretizations for Elliptic Problems with Tensor Coefficients

We present a mimetic discretization in 2-D for a heterogenoeus elliptic equation with application to reservoir simulations. The method discussed belongs to a new class of methods called mimetic. Standard methods are applied by discretizing the differential equations directltly. One disadvantage is that the selected discretization may have little connection with the underlying physical problem. Mimetic methods in the other hand begin by first discretizing the continuum theory underlying the problem. By "discretizing the continuum theory" we mean that mimetic methods initially construct a discrete mathematical analog of a relevant description of continuum mechanics. Typically this description takes the form of a physical conservation or constitutive law. The discrete form of the conservation or constitutive law constrains the structure that discrete operators can take. After building discrete operators that obey the discrete physical law, these mimetic operators can be used to construct a discrete analog of the system of partial differential equations or Integral equations. This yields a mimetic discretization for the boundary value problem which automatically satisfy the discrete version of the physical law.

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CP1
Compressible Two-Pressure Two-Phase Flow Models

A central problem for compressible two-pressure two-phase flow models is closure, or the proper definition of averages of nonlinear term. We propose here a new closure, which appears to be unique in satisfying a number of fundamental physical requirements. An entropy inequality is derived from an assumed positivity of the entropy of averaging. The closures proposed are new and validation against simulation data is presented. The simulation data is validated separately against laboratory experiments.

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CP1
A Fourth Order Ppm Finite Volume Based Spectral Deferred Correction Method For Solving Conservation Laws

We present a new fourth order PPM (Piecewise Parabolic Method) finite volume based SDC (Spectral Deferred Correction) method for solving conservation laws. We use PPM framework to define edge averaged quantities which are used to evaluate fluxes. We use a fourth order Spectral Deferred Correction technique to update the state variables in time. The method is tested by solving variety of problems. The results indicate that we achieved fourth order of accuracy in time and space when the flow is smooth. The results also demonstrate the shock capturing ability of our newly proposed technique when the flow experiences shock waves.

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CP1
Characteristic Finite Element Methods for Convection-Dominated Transport Equations

We shall examine theoretical features of commonly used characteristic finite element methods for convection-dominated transport equations for fluid flows in porous media, e.g., Galerkin-Lagrangian methods and Eulerian-Lagrangian localized adjoint methods. Efficient implementation of these methods on unstructured meshes will be presented. We shall also present some numerical experiments and discuss issues about combining characteristic tracking with adaptive finite methods.

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CP1
Initial Decay of Velocity Fluctuations of a Sedimenting Suspension in a Large Container

For a well-stirred suspension of particles settling in a large container, the initial decay of the velocity fluctuations is governed by the equations governing the settling of a viscous fluid with variable density. This model makes specific predictions for the decay of large scale density fluctuations, the density gradient resulting from the decay and the nature of fluctuation enhanced sedimentation.

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CP1
Well-Posed and Stable Boundary Treatment for the Navier-Stokes Equations

A well-posed set of boundary conditions for the three-dimensional Navier-Stokes equations based on the Euler characteristics is derived. The boundary treatment is local, and allows for inflow and outflow at the same boundary. A stable implementation of these boundary conditions is possible with the Simultaneous Approximation Term technique for numerical schemes satisfying a summation-by-parts property. Numerical computations using a high-order finite difference scheme corroborate the theoretical results.

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CP1

Entropy Stable Approximations of Navier-Stokes Equations with No Artificial Numerical Viscosity

We construct a new family of entropy stable difference schemes which retain the precise entropy decay of the Navier-Stokes equations. To this end we employ the entropy conservative differences to discretize Euler convective fluxes, and centered differences to discretize the dissipative fluxes of viscosity and heat conduction. The resulting difference schemes contain no artificial numerical viscosity in the sense that their entropy dissipation is dictated solely by viscous and heat fluxes. Numerical experiments provide a remarkable evidence for the different roles of viscosity and heat conduction in forming sharp monotone profiles in the immediate neighborhoods of shocks and contacts.

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CP2

The Influence of Parametric Forcing on the Non-Equilibrium Dynamics of Wave Patterns

We study the effect of heterogeneities on the non-equilibrium dynamics of wave patterns in the framework of a complex Ginzburg-Landau equation with parametric forcing dependent on the coordinate and time. Wave solutions quasi-periodic in space and time are found, and their stability is investigated. Numerical simulations reveal a strong suppression of the intermittent chaos by the parameter modulation. The theory is applied to the effect of surface topography on the dynamics of thermal Rossby waves.

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CP2

The Permutation Entropy of Information Sources and Interval Maps

Permutation entropy quantifies the diversity of possible orderings of the values a random or deterministic system can take. It can be shown that the measure-theoretic and permutation entropy rates are equal for ergodic finite-alphabet information sources and that the same holds for deterministic dynamical systems defined by ergodic maps on n-dimensional intervals. The cases of non-ergodic finite-alphabet sources and ergodic arbitrary sources will be also considered.

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CP2

Noise-Induced Cellular Patterns on Circular Domains

We study the effects of thermal noise in a stochastic formulation of a generic example, the Kuramoto-Sivashinsky equation, of a pattern-forming dynamical system with two-dimensional circular domain. Numerical integration reveals that the presence of noise increases the propensity of dynamic cellular states, which seems to explain the generic behavior of related laboratory experiments. Most importantly, we also report on observations of certain dynamic states, homoclinic intermittent states, previously only observed in physical experiments.

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CP2

Patterns on Growing Square Domains Via Mode Interactions

We consider reaction-diffusion systems on growing square domains with Neumann boundary conditions (NBC). We study transitions between two types of squares and transitions between squares and stripes using mode interactions for bifurcation problems with $D_4 + T^2$ symmetry (*hidden symmetries*) and the symmetry constraint imposed by

NBC. We obtained surprising results: the transition from squares to stripes in NBC can go through time periodic states, and there are differences between periodic boundary conditions and NBC problems.

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CP2

Linear Pattern Generation and Fibonacci Numbers

We will show the connection between expected time of simple linear patter generation and a sum of series involving Fibonacci numbers as well as generalizations of this result. This result is unexpected spinoff of investigation into distribution and expected times of simple linear patterns generation, the so called success runs, in the theory of discrete Markov Chains.

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CP2

A Rigorous Formalism of Information Transfer Between Dynamical System Components

We put the concept of information transfer on a rigorous footing and establish for it a formalism in the framework of a dynamical system. The resulting transfer measure possesses a property of directionality as emphasized by Scrheiber (2000); it also verifies the transfer measure for 2D systems,which was obtained by Liang and Kleeman (2005) through a different avenue.Connections to classical formalisms are explored and applications presented.We find that, in the context of the baker transformation, there is always information flowing from the stretching coordinate to the folding cordinate, while no transfer occurs in the opposite direction; we also find that, within the Henon map system, the transfer from the quadratic component to the linear component is of a simple form as expected on physical grounds.This latter result is unique to our formalism.

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CP3

A Drug-Drug Interaction Parameter Estimation Problem

A two drug interaction is usually predicted by individual drug pharmacokinetic. An innovative drug-drug interaction prediction method based on a three-level hierarchical Bayesian meta-analysis model is developed that includes a Monte Carlo Markov chain pharmacokinetic parameter estimation procedure. Underlying the parameter estimation procedure is a fast integration method of the stiff pharmacokinetic equations. In this presentation, we report the results of the fast integration method and comparisons with standard stiff solvers. We also discuss the interrelation between the Monte Carlo Markov chain pharmacokinetic parameter estimation procedure and the numerical integration scheme.

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CP3

The Role of Neuronal Coherence in Attentional Processing

Rhythmic synchronization of large groups of neurons is believed to be a common occurrence in the central nervous system, reflected in the oscillations in the EEG. Attentional processing is among the mental activities particularly associated with oscillations. I will present numerical simulations of networks of model neurons that suggest possible functional roles for rhythmic synchronization in attentional processing. This is joint work with Nancy Kopell and Steven Epstein.

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CP3

An Estimation Method for the Outbreak of An Infectious Disease

Recent concerns of a natural or manufactured (bioterrorism) outbreak of an infectious disease give rise to the desire for an algorithmic approach to early detection. The availability of field data, the tools of mathematical biology, and signal estimation techniques can be combined to produce such a method. By fusing a simplified SIR model, data from the Childrens Hospital of Boston bioinformatics group, and the Kalman filter, a methodology to determine the outbreak of a simulated epidemic is presented.

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CP3

A Dynamical Model of Human Immune Response to Influenza A Virus (IAV) Infection

We present time courses of model variables of the IAV infection in an individual, explore the effect of initial viral load and perform sensitivity analysis to explore which parameters influence the onset, duration and severity of infection. Immune memory is modeled by a new variable that quantifies the antigenic distance between the virus and the existing antibodies.

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CP3

Disease Modeling to Assess Outbreak Detection and Response

Bioterrorism is a serious threat that has become widely recognized since the anthrax mailings of 2001. In response, one national research activity has been the development of biosensors and networks thereof. A driving factor behind biosensor development is the potential to provide early detection of a biological attack, enabling timely treatment. This presentation introduces a disease progression and treatment model to quantify the potential benefit of early detection. To date the model has been used to assess responses to inhalation anthrax and smallpox outbreaks.

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CP3

Regulation Mechanisms in the Immune System

We model interactions among effector and regulatory T cells during an immune response to two simultaneous targets to show that the system discriminates based on target behavior and not only TCR affinity. The model affirms the necessity of regulatory cells for self-tolerance, but also shows that low amounts do not hinder, but enhance strong responses by inducing T cell contraction and emigration from the lymph node, leading to rapid target elimination.

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CP3

Nonlinear Dynamics of a Double Bilipid Membrane

The nonlinear dynamics of a double biological membrane that consists of two coupled lipid bilayers, typical of some intra-cellular organelles such as mitochondria, is studied. A phenomenological free-energy functional is formulated in which the curvatures of the two parts of the double membrane are coupled to the lipid densities. The derived nonlinear evolution equations for the double membrane dynamics are studied analytically and numerically. The linear stability analysis is performed and the domain of parameters is found in which the double membrane is stable. For the parameter values corresponding to an unstable membrane, we perform weakly nonlinear analysis and numerical simulations that reveal various types of complex dynamics.

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CP4

Simple Adaptive Synchronization of Chaotic Systems with Random Components

Practical systems usually possess random components. Random components often affect the robustness of synchronism and must be taken into consideration in the design of synchronization. In the present study, we assume that the system satisfies the Lipschitz condition, and the random component is uniformly bounded. By the partial stability theory, we are able to prove that two simple adaptive variable structure controllers achieve synchronization of chaotic systems. Moreover, we discuss how the controllers can be modified to eliminate the undesired phenomenon of chattering. The Duffing two-well system and the Chua circuit system are simulated to illustrate the theoretical analysis.

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CP4

An Extension of the Cumulative Residual Entropy

Cumulative Residual Entropy(CRE) is a new measure of entropy defined for positive random vectors. Since negative random variables play important roles in many cases, we generalized the definition of CRE to negative random variables. Several nice properties of new CRE and examples will be addressed in the talk.

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CP4

Lyapunov Optimizing Control with Trajectory Following Minimization: Analysis and Application in the Optimal Control Setting

Lyapunov optimizing control merges Lyapunov stability theory with function minimization to generate feedback controls. Trajectory following minimization algorithms locate the minimizer by solving special systems of differential equations. We combine these techniques to create suboptimal, closed-loop controls in the optimal control setting. Of particular interest are systems where bang-bang or bang-intermediate control may enter the solution. Target stability, time scale analysis, and chatter considerations yield new theoretical and practical results.

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CP4

Feedback Control of a Subcritical Instability

A nonlinear feedback control is needed for stabilization of systems which are subject to subcritical instabilities and blow up. Near the linear instability threshold such systems are described by a Ginzburg-Landau equation with a negative Landau coefficient. We show that a feedback control can suppress the blow-up and stabilize a stationary pulse solution in the weakly nonlinear regime. The dependence of the pulse stability on the gain and time-delay parameters is studied analytically and numerically.

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CP4

Monitoring Gas Turbines Via Their N-Dimensional Analog Signal Representation

Gas turbines are usually monitored by a large set of analog signals. The operator must, at any time, be able to judge whether - the system is in an undesirable state or not (detection) or - any such event will occur in the near future (forecast). The information available is, after appropriate data transformation, a subset of the n-dimensional hypercube of length 1. State of the art statistics and pattern recognition methods will be studied to study the n-dimensional hypercube.

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CP4

Feedback Control of Pattern Formation

Global feedback control of spatially-regular patterns described by the Swift-Hohenberg (SH) equation is studied. Two cases are considered: (i) the effect of control on the competition between roll and hexagonal patterns; (ii) the suppression of sub-critical instability by feedback control. In case (i), it is shown that control can change the stability boundaries of hexagons and rolls. In case (ii), the feedback control suppresses the unbounded solutions of a sub-critical SH equation and leads to the formation of spatially-localized patterns.

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CP4

A Reduced Basis Domain Decompositon Method for Optimal Control

A spatial domain decomposition method for certain optimal control problems is proposed. A reduced basis solution of linear-quadratic parabolic optimal control problems at subdomain interfaces provides significant reduction in computing time and storage requirements. The problem is decomposed into smaller optimal control subproblems defined on spatial subdomain-time cylinders coupled by suitable transmission conditions which are approximated through balanced truncation model reduction. The approach is highly parallel and also provides error estimates.

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CP5

The Retraction Algorithm for Factoring Banded Symmetric Indefinite Matrices

An algorithm will be presented for factoring symmetric banded matrices that may be indefinite. The algorithm preserves symmetry and band structure and bounds the element growth in the transformed matrices. It requires less space and fewer multiplications than unsymmetric Gaussian elimination. The problem might arise when finding eigenvalues of a banded symmetric system and was motivated by an inverse problem in determining the chemical composition of an optical fiber wrapped around a spool.

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CP5

Jacobian-Free Newton-Krylov for Steady-States and Limit-Cycles of Time-Steppers

A Jacobian-Free Newton-Krylov method for computing steady-state and limit-cycle solutions to existing time-stepping software is tested for a two-dimensional, lid-driven

and thermally-driven fluid cavity. Comparisons to existing methods, some of which are unavailable to truly legacy time-steppers, are made over a variety of algorithmic and physical, including periodically-forced problems. The J-F N-K method is robust and competitive, improving by factors of an order of magnitude or more over conventional time-stepped alternatives. Due to its matrix-free nature, preconditioning, essential at large-scales, is nontrivial.

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CP5

The Effect of Dangling Nodes on Google's PageRank

The Google search engine makes use of a stochastic matrix to model the Internet. WebPages that have no out-links, such as an image file, are known as dangling nodes. These pages present a problem in the forming of the stochastic Google matrix. The calculation of PageRank relies on the stochastic nature of the Google matrix. Specifically, the PageRank assigned to each webpage is related to the order in which pages are returned during web query. Our goal is to view how changes in the treatment of dangling nodes affects the value of PageRank.

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CP5

Cost-Effectiveness of Fully Implicit Moving Mesh Adaptation

The cost-effectiveness of moving mesh adaptation is studied in a number of tests. We propose a method that is based on two established modern techniques. First, we use a moving mesh approach based on variational grid adaptation and error minimization. We consider the classic Brackbill-Saltzmann-Winslow method. Second, we discretize the model equations for grid and physics using a conservative finite volume method and we solve the resulting equations with a preconditioned inexact Newton-Krylov method.

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CP5

Ten Digit Algorithms

A Ten Digit Algorithm is a computer program that solves a numerical problem and satisfies three conditions:

Ten digits,
Five seconds,
And just one page.

These conditions may seem like gimmicks, but in fact, this is a style of programming with much to recommend it for most people doing scientific computing, most of the time. Ten Digit Algorithms can

- improve our publications
- speed up program development
- make our numerical methods faster
- make our scientific results more reliable
- facilitate comparisons of ideas and results
- add focus to the classroom
- add zest to our field

A dozen examples will be presented.

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CP6

Mathematical Analysis of Effector Caspase Amplification in the Death Receptor Network in Single-Cells

A proposed mechanism of ligand-induced single-cell rapid all-or-none death is positive feedback in the apoptotic network. However, this hypothesis is not supported experimentally in HeLa cells. Apoptosis is described by an experimentally verified, mass-action ODE model, which indicates that in single HeLa cells, the mitochondrial death pathway is responsible for rapid, all-or-none apoptosis. As a corollary of Singular Perturbation model reduction, a threshold parameter is identified that when crossed, initiates fast, all-or-none mitochondrial cell death.

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CP6

Modeling Competition Between Inhibiting and Purely Cannibalistic Species

Much research has been done on modeling population dynamics of the beetle species *Tribolium castaneum*, which heavily regulates population growth through cannibalism of eggs and pupae. Recent experimental work has shown that several other species of *Tribolium* also manage population size through *inhibition* - larvae are prevented from entering the pupal stage for long periods of time due to excessive contact with other individuals in the population. A discrete model of competition between two distinct stage-structured species is developed and analyzed.

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CP6

Survival Prediction Via Gene Expression Profile in Gastric Cancer Patients after Surgical Resection

This study was conducted to characterize gene expression profile and create prediction model of survival in patients with surgically curable gastric cancer. 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 survival and survival curves are presented showing the prediction power.

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CP6

Mathematical Epidemiology of HIV/AIDS in Cuba

HIV is a global problem with an estimated 40 million infected worldwide. Population infectivity estimates range as high as 8.5% for Sub-Saharan Africa, and as low as less than 0.1% for East Asia and Australia/New Zealand. Cubas infectivity is estimated at less than 0.1% despite its status as a relatively resource-poor nation. The two main methods for detection of HIV/AIDS cases in Cuba are "random testing and contact tracing. When modeling the HIV transmission dynamics for Cuba we must include these two detection methods. As the detection equipment is costly and depends on biotechnological advances, the testing rate can be changed by many external factors. Therefore, our model includes time-dependent testing rates. By comparing our model to the 1986-2000 Cuban HIV/AIDS data and previous models, we show that socioeconomic aspects are an important factor in determining the dynamics of the epidemic. The understanding of Cuban HIV/AIDS infectivity dynamics may assist the design of preventive and reactive measures to HIV in countries with high HIV prevalence.

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CP6

Determining Environmental Conditions for Successful in-Vitro Maturation of Mammalian Oocytes

Harvesting of immature oocytes (eggs) and successful maturation in the laboratory would be a significant breakthrough in the field of assisted reproduction techniques. Success is believed to depend on the ability to mimic the nutritional environment that pertains within the body in the ovarian follicle surrounding the oocyte, which is difficult to determine experimentally. We describe mathematical modelling, using experimental micronutrient data, which is aimed at increasing our understanding of the in-vivo oocyte environment.

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CP6

A Model of the Opiate Using Career

The results of the first Irish attempts to extend mathematical disease modelling techniques to the drug-using career are presented; a simple deterministic compartment model of the drug-using career, incorporating an observed cycle in and out of treatment, is developed and analysed. R_0, the basic reproduction number, is derived for this model. Existence and stability of the disease-free and endemic equilibria of the model are examined and the associated implications for the drug-using career are discussed.

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CP7

On the Existence of a Center Manifold and Lie Symmetries for a Model of the Growth-Death Kinetics of *Staphylococcus Aureus* in Bread

Using center manifold theory and Lie symmetries, we investigate a quasi-chemical model for the growth-death kinetics of *Staphylococcus aureus* in bread. Food scientists at the Natick Soldier Center developed this model to numerically determine shelf life of packaged sandwiches for the military. Our new results proving the existence of a center manifold and Lie symmetry for this model qualitatively predict the behavior of solutions and extend the original papers numerical results.

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CP7

A State-Dependent Delay Equation for Microvascular Bloodflow

We discuss a novel state-dependent delay equation for a simple model of microvascular bloodflow based on a transformation of the governing partial differential equations. We show that instability of the equilibrium state is possible in a variety of simple networks, including those with 2, 3, and 4 nodes. We explore the resulting nonlinear dynamics, and discuss the relevance to in vivo and in vitro experiments.

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CP7

Kink-Antikink Nonlinear Wave Collisions in a Cubic Klein-Gordon Equation: The N-Bounce Resonance and the Separatrix Map

We study a finite-dimensional "collective coordinates" model. We use dynamical systems and matched asymptotic expansions to explain the two-bounce resonance phenomenon originally investigated in collisions between kink and antikink traveling waves by Campbell. We derive the critical relative velocity below which the interacting kinks have complex behavior, which agrees with our accurate numerical simulations. We derive a separatrix map that explains the complex fractal-like dependence on initial velocity for kink-antikink interaction.

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CP7

Monotonicity, Boundedness and Periodic Character of the Positive Solutions of a Rational Difference Equation

It is our goal to investigate the long term behavior of the solutions of the following difference equation: x[n+1]=(A[n]x[n-1])/(1+x[n]) , n=0,1,2,...... where A[n] is a periodic sequence of positive real numbers. We will examine how the different periods of the sequence and the relationship of the terms of the sequence affect the long term behavior of the solutions.

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CP7

An Optimization Algorithm for the Identification of Biochemical Network Models

We introduce an Evolutionary Algorithm (E.A) for the systematic finding of an optimal robust discrete model for the description of biochemical networks. Our algorithm takes as input discretized time series as well as information provided by the method presented in [1], about the structure of all possible solution discrete models for the reverse engineering problem. We employed tools from computational algebra in order to provide a simple description of the mutation rules of the E.A., and simultaneously to provide a reduction of the search space. [1] A. Jarrah, R. Laubenbacher, B. Stigler, M. Stillman, Reverse-engineering of finite dynamical systems. Preprint.

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CP7

Particle Tracking in Three-Dimensional Flows: Evolution and Refinement of a Smooth Surface

An initial surface represented parametrically on a domain in the (u, v) plane is evolved under the flow map for a system of three ODEs. Given a triangulation on the points

in (u, v) space, the C^1 surface is represented as the Clough-Tocher interpolant, a piecewise bicubic requiring no more than first derivatives. We present a technique for refining the surface representation when it is determined that the accuracy of the interpolation is no longer sufficient.

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CP8

Limits for Szego Polynomials in Frequency Analysis

We characterize limits for orthogonal Szego polynomials of fixed degree k, with respect to certain measures on the unit circle which are weakly convergent to a sum of $m < k$ point masses. Such measures arise, for example, as a convolution of point masses with an approximate identit. It is readily seen that the underlying measures in two recently-proposed methods for estimating the m frequencies of a discrete-time trigonometric signal using Szego polynomials are of this form.

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CP8

Block Krylov Subspace Methods for Eigenvalue and Svd Problems

For the eigenvalue problem, we have developed a block Householder restarted Arnoldi method that is based on augmentation of Krylov subspaces. We will provide examples and discuss the connection between a block and single vector implementation. The SVD algorithm is a restarted block Lanczos bidiagonalization method, which is based on augmentation of Ritz vectors or harmonic Ritz vectors by block Krylov subspaces. MATLAB codes are available for both methods.

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CP8

Computing the Zeros of Truncated Fourier Series and Chebyshev Polynomial Series: Roots of Polynomials in Spectral Form

We derive a companion matrix method for finding the zeros of a trigonometric polynomial. We show how existing companion matrix methods for orthogonal polynomials, which reduce rootfinding to a standard eigenvalue problem, can be accelerated to exploit parity symmetries, and similarly for truncated Fourier series. Alternatively, eigenvalue-solving methods for rootfinding can be replaced by subdivision algorithms that exploit rigorous error bounds when the function whose roots are sought is a finite Chebyshev or Fourier series.

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CP8

Generalized Symmetry Preserving Singular Value Decomposition

Determining symmetry within a collection of spatially oriented points is a problem that occurs in many fields. In these applications, large amounts of data are generally collected, and it is desirable to approximate this data with a compressed representation. In some situations, the data is known to obey certain symmetry conditions, and it is profitable to preserve such symmetry in the compressed approximation. We accomplish this task by providing a symmetry preserving singular value decomposition.

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CP8

On Ill-Conditioning of Google's PageRank Algorithm

Google is an extremely efficient search engine. The main ingredient of Google's algorithm is PageRank. In their original paper : "The PageRank Citation Ranking: Bringing Order to the Web", Page et al. show that ranking the web pages boils down to solving a huge eigenvalues problem $Ax = x$ where A is a matrix which represents a graph related to the web. In our talk, we would like to show that this eigenvalues problem is highly ill-conditioned. Small change in the matrix can result in huge change in the solution vector. We will demonstrate that due to this fault, PageRank can give unrealistic results.

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CP8

The Reduction to Hamiltonian Schur Form Explained

The Linear-Quadratic Gaussian problem of control theory can be solved by computing the stable invariant subspace of a Hamiltonian matrix. For 25 years it has been an open problem to produce a backward-stable algorithm that solves the problem in a structure-preserving way by computing the Hamiltonian Schur form. Recently Chu, Liu, and Mehrmann proposed such an algorithm. We will present an alternate derivation of their algorithm that explains it in terms of swapping blocks of eigenvalues in the square of the Hamiltonian matrix.

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CP9

Limit Behavior of the Optimal Value of Random Multidimensional Assignment Problem

The Multidimensional Assignment Problem (MAP) is a hard combinatorial optimization problem that arises in the areas of data association, target tracking, resource allocation, etc. We elucidate the question of limit behavior of the optimal value of large-scale MAP whose assignment costs are iid random variables from a broad class of probability distributions. Moment convergence and almost sure

convergence of its optimal value are investigated, and converging asymptotical bounds for the expected optimal cost are constructed.

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CP9
Radiation Source Inversion From Detector Data

The determination of a radiation source in a closed domain given only surface detector data is formulated as an inverse problem for the source fields. In particular, the mathematical formulation is expressed as a regularized PDE-constrained optimization problem for the unknown emission field (and possibly density and absorption fields), where the PDE constraints are the equations for the discretized specific intensities obtained from the radiation transfer equation. Forward calculations of the radiation field on a finite-element mesh are presented, as well as preliminary inverse calculations based on the specification of a Lagrangian objective function, the introduction of Lagrange multipliers for the PDE constraints and a solution of the KKT necessary conditions. The ability to detect sources from non-intrusive detector measurements has various security applications, including the identification of radioactive devices in transport containers.

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CP9
Spatiospectral Localization on a Sphere

We pose and solve the analogue of Slepian's time-frequency concentration problem on the surface of the unit sphere, to determine an orthogonal family of strictly bandlimited functions that are optimally concentrated within a closed region of the sphere. Such a basis of simultaneously spatially and spectrally concentrated functions should be a useful data analysis and representation tool in a variety of geophysical and planetary applications, as well as in medical imaging, computer science, cosmology and numerical analysis. (SIAM Review, in press, 2006).

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CP9
A Constrained Minimization Algorithm for Electronic Structure Calculation

One of the fundamental problems in electronic structure calculation is to determine wave functions associated with the minimum total energy of large atomistic systems including nanoscale structures. A constrained minimization algorithm for solving such a problem will be presented in this talk. The performance of these algorithm wil be compared with the commonly used Self Consistent Field (SCF) iteration, a fixed point iteration applied to a non-linear eigenvalue problem characterizing the 1st-order necessary condition of the minimization problem.

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CP9
Smooth Optimization for Sparse Semidefinite Programs

We show that the optimal complexity of Nesterov's smooth first-order optimization technique is preserved when the function value and gradient are only computed up to a small, uniformly bounded error. This means that only a partial eigenvalue decomposition is necessary when applying this technique to semidefinite programs, thus significantly reducing the method's computational and memory requirements. This also allows sparse problems to be solved efficiently.

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CP10
Vacuum Formation in Multi-Dimensional Compressible Flows

It is well known that vacuum formation can occur for inviscid compressible flows. However, for viscous compressible flows, governed by the Navier-Stokes equations, vacuum formation in the multidimensional case is an open question. The analytic difficulties associated with this problem translate into numerical difficulties requiring the use of a highly accurate method. Using a spectrally accurate collocation method, we show that vacuum formation does occur under certain conditions.

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CP10

Analysis and Computation of the Paraxial Wave Equation

We present analysis and computation of an initial value problem for the Paraxial Wave Equation. The computation is based on the Galerkin Method and Hermite-Gauss eigenfunctions.

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CP10

A New Spectral Dynamical Core for the High-Resolution Global Atmospheric Model

We are developing a new spectral dynamical core for the global atmospheric model, aiming to improve the computational efficiency of the model with the maximum truncation wavenumber T959. The core is equipped with a reduced Gaussian grid and a unique semi-Lagrange advection scheme. The model will be used for the research of global warming at MRI and for daily weather forecasts at JMA. The specifications and the performance of the model will be presented.

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CP10

Seismic Sources and Waves Using Finite Differences

We present a finite difference method for the 2nd order elastodynamic equations. We avoid stability problems by using a special treatment of the discretized equations close to the boundary. The method is second order accurate, and energy conserving. Seismic events often have singular behavior in space. We describe observed convergence properties of the numerical solution and improvements in modeling of the singular parts of the source. We will give examples of simulations of seismic events in the San Francisco region.

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CP10

High-Precision Solution of the Poisson Equation by a Redundant Basis

We present a procedure for solving the Poisson equation using a redundant set of eigenfunctions. The procedure involves a uniform grid, and an overcomplete dictionary comprising sines and cosines. The right-hand side of Poisson's equation is preconditioned with a set of cosine basis functions determined by its boundary behavior; then a standard spectral solver is applied to the preconditioned equation. The procedure is highly accurate, and extendable to other elliptic problems. Several examples will be given.

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CP11

On Trivial Solutions to the Steady States of Kuramoto-Sivashinsky Equations

In this talk we consider the integrated Kuramoto-Sivashinky equation (KSE). We show that the only locally integrable steady state solutions on R^N, $N = 1, 2$, are the trivial constant solutions. However, for $N = 3$ D. Michelson was able to construct, using a computer assisted proof, a non-trivial radial steady state solution. It is worth mentioning that in the particular case of periodic boundary conditions one can easily show that the only steady state solutions to the integrated KSE are the constant solutions, for all $N = 1, 2, \cdots$.

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CP11

Teleprojective Integrators for Atomic Kinetics Problems

Projective integrators are explicit methods that efficiently exploit the multiscale features that are characteristic of stiff systems. We will introduce these methods, and describe their use on stiff atomic kinetics problems. An important outcome is that the new integrators, when combined with a telescopic projective inner integrator, can result in fully-explicit methods with adaptive outer step size selection and solution accuracy comparable to those obtained by implicit integrators.

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CP11

A Modified-Leray-α Subgrid Scale Model of Turbulence

Inspired by the remarkable performance of the Leray-α (and the Navier-Stokes alpha (NS-α), subgrid scale model of turbulence as a closure model to Reynolds averaged equations (RANS) for flows in turbulent channels and pipes, we introduce another subgrid scale model of turbulence, the Modified Leray-α (ML-α) subgrid scale model of turbulence. The application of the ML-α to infinite channels and pipes gives, due to symmetry, similar reduced equations as the Leray-α and the NS-α. As a result the reduced ML-α model in infinite channels and pipes is equally impressive as a closure model to RANS equations as the NS-α.

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CP11

Existence and Uniqueness of Viscous/Inviscid Interactions Using Interfacial Data in Navier-Stokes Equations.

Navier-Stokes equations are often used in computations of static/dynamic models which require an understanding of interfacial interaction between the viscous/inviscid regions. This paper will discuss the following (i) existence/uniqueness of system solutions (ii) system solutions limited by two sub-problems with sub-domains defined by Xus theory [SIAM J. Numerical Analy., 38, 4, 2000, 1217]. Also discussed will be methods of numerical stability, faster computation characteristics and, flow regimes with extended separation regions localized within viscous sublayers.

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CP11

Double Periodicity in the Gledzer Shell Model of Turbulence

The shell model of turbulence introduced by Gledzer with six real variables is studied numerically by using Mathematica. Doubly periodic stable solutions are observed in the space of the first three modes. The complex representation of the two successive values of the first mode in the Poincare section gives the return map of its argument. The function has many Fourier components but the bifurcation diagram is similar to that of the sine circle map.

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CP11

Numerical Modeling of Fluid Mixing for Laser Experiments and Supernova

We have conducted front tracking simulations for axisymmetrically perturbed spherical explosions relevant to supernovae as performed on NOVA laser experiments, with excellent agreement with experiments. We have extended the algorithm and its physical basis for preshock interface evolution due to radiation preheat. Our second focus is to study turbulent combustion in a type Ia supernova (SN Ia) which is driven by Rayleigh-Taylor mixing. We have extended our front tracking to allow modeling of a reactive front in SN Ia. Our 2d axisymmetric simulations show a successful level of burning.

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CP12

Modeling the Effects of 4-Methylimidazole Exposure

The chemical 4-Methylimidazole (4-MI) is used in the manufacture of a variety of pharmaceuticals as well as photographic and agricultural chemicals, and its toxicity has been under investigation by the National Toxicology Program. In support of this study, a physiologically based pharmacokinetic model of the uptake and disposition of 4-MI in rats and mice was developed to predict the tissue doses of 4-MI resulting from intravenous and oral exposure. Acute exposure data were used to gain information needed for the model. The model was then used to predict chronic exposures, and the numerical results were compared to chronic data.

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CP12

Calculations of Oxygen Transport in Muscle Using Simulated and Measured Capillary Network Geometry

The details of O_2 transport heterogeneity in muscle, particularly during exercise, are difficult to obtain experimentally. Therefore, a computational model is used to study muscle O_2 distributions under resting and exercising conditions, based on measurements of resting capillary hemodynamics and red cell oxyhemoglobin saturation. Blood flow and O_2 transport models are described, and results are presented of steady-state O_2 transport simulations using both simulated capillary networks (parallel arrays) and 3D networks reconstructed from experimental data.

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CP12

Einstein Relation Approach to Protein Folding Dynamics

We propose a protein folding simulation approach (based on energy type partition and Einstein Relations for constrained movements) as the important key for understanding of protein shape change dynamics. Lagrange methods ensure that the simultaneous minimization of two or more energy forms is describable in terms of the free energies, gradients or forces. Interesting point is that a structural free energy gradient exactly balances an electrical ensemble gradient leading to an infinite mobility.

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CP12

Using Stochastic Partial Differential Equations to Model and Treat the Seizing Human Cortex

We discuss a mathematical model of the seizing human cortex. The model consists of fourteen stochastic partial differential equations (SPDEs). We illustrate the bifurcations in a simplified formulation of the model and relate these results to traveling wave solutions of the complete SPDEs system. We compare the model results with electrocorticogram recording from a human subject and show that the simulated and observed data agree. Finally, we suggest techniques to abort a seizure.

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CP12

Morphogen Gradient Mechanisms in the Developing Brain

Morphogens are secreted signalling molecules that influence cell fate specification, proliferation, and the activity of induced genes on the basis of their spatio-temporal concentrations. Understanding morphogen gradient interpretation mechanisms "[Ashe HL, Briscoe J. The interpretation of morphogen gradients. Development. 2006 Feb;133(3):385-94.]" at the cellular level is important to understanding morphogen functioning. We focus on cellular mechanisms in the developing brain "[Monuki ES, Porter FD, Walsh CA. Patterning of the dorsal telencephalon and cerebral cortex by a roof plate-Lhx2 pathway. Neuron. 2001 Nov 20;32(4):591-604.]" that enable bistable switch-like behavior of the induced genes. We identify several bistable switch-like candidates in the developing brain based on a) morphogen and induced gene expressions, and b) regulatory pathway network structures. The analysis of the complex dynamics is done with the help of logical and ODE-based methods "[THOMAS, R. and KAUFMAN, M., "Multistationarity, the basis of cell differentiation and memory. II. Logical analysis of regulatory networks in terms of feedback circuits.", Chaos 11, (2001) 180-195.]","[THOMAS, R. and KAUFMAN, M., "Multistationarity, the basis of cell differentiation and memory. I. Structural conditions of multistationarity and other nontrivial behavior.", Chaos, 11 (2001) 165-179.]".

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CP12

Evolution Equations of Biological Structures Formed in Cholesterol Crystallization Processes

In gallbladder bile, its three major components, bile salts, cholesterol and phospholipids, under certain conditions, conglomerate and evolve to form a wide variety of structures: filaments, helices, membranes, and tubules, to name a few. These structures, believed to have a cholesterol core and phospholipid surfaces, have thicknesses on the nanoscale while their contour length is on the micron scale. We present sets of evolution equations that describe the shape of the centersurface of these structures, the surface boundaries, and the local average phospholipid concentrations along the surface. Comparisons of our theory with our ongoing experimental program are presented.

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CP13

High-Frequency Cavity Modes: Fast Methods and Quantum Chaos

The 'drum problem'—finding the eigenmodes of the Laplacian in a cavity—has a long history and a wealth of applications. At high wavenumber k this becomes a challenging multiscale problem. New variants of the Method of Particular Solutions (global basis representations, boundary matching) allow $O(k)$ tighter eigenvalue inclusion bounds, and $O(k)$ more efficient calculation of eigenmodes. I discuss the recent convergence with the work of Betcke-Trefethen, and present a large-scale study of eigenmode equidistribution in 'quantum chaos'.

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CP13

Closure Conditions for Convergence of Discrete Approximations in Optimal Control

While Eulerian type discrete approximations to optimal control problems have been widely studied with roots going back to Eulers own derivation of the Euler-Lagrange equations, higher-order approximations are of recent vintage. Higher-order approximations are computationally more attractive, but they do not naturally offer the elegant control-theoretic properties of Eulerian approximations. In recent years, Hager has offered a class of nontraditional Runge-Kutta methods for optimal control that is based on commuting the operations of dualization and discretization. These unconventional Runge-Kutta methods must satisfy closure conditions that lead to a new class of symplectic methods. While Hagers closure conditions are in the primal space, the closure conditions for the Legendre pseudospectral (PS) method are in dual space. Unlike Hagers conditions, PS approximations to optimal control problems converge without an imposition of closure conditions; however, closure conditions are still necessary to select the proper sequence of discrete multipliers that converge to their continuous-time counterparts.

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CP13

Some Results Concerning the Stability of Staggered Multistep Methods

Staggered multistep methods are quite useful for approximating solutions to wave equations. In this talk, we prove two theoretical results concerning staggered finite difference methods. First, we give an extension of Dahlquists First Stability Barrier to staggered finite difference methods. Secondly, we prove that staggered backwards differentiation methods are unstable for orders greater than four.

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CP13

A Krylov-Karhenun-Loeve Moment Equations Approach for Uncertainty Assessment

The Karhenun-Loeve moment equation (KLME) method has emerged as a competitive alternative for subsurface uncertainty assessment since it involves simulations at a lower resolution level than Monte Carlo. Algebraically, the KLME method reduces to the solution of several linear systems with different right hand sides. We propose a new family of block deflated Krylov iterative to efficiently compute different orders and statistical moments. Numerical results are encouraging to extend the approach to other numerical/industrial applications.

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CP13

How Rare Are Large Growth Factors?

The growth factor of a matrix quantifies potential error growth when a linear system is solved by Gaussian elimination with partial pivoting. While the growth factor has a maximum of 2^{n-1} for an $n \times n$ matrix, the occurrence of matrices with exponentially large growth factors is extremely rare. We implemented a multicanonical Monte Carlo method to explore the tails of growth factor probability distributions for random matrices. Our results attain a probability level of 10^{-12}.

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CP13

Is Gauss Quadrature Better Than Clenshaw-Curtis?

Gauss quadrature is famous, elegant, and in a certain sense optimal, but determining the Gauss nodes and weights is difficult for large n. By contrast the nodes and weights for Clenshaw-Curtis quadrature are given by explicit formulas and trivially implemented with the FFT, even if n is as large as 10^6. But doesn't Clenshaw-Curtis require twice as many points for a given accuracy? For most integrands, the surprising answer is no. This observation was made by O'Hara and Smith in 1967 but seems to have been forgotten. We explain what is going on.

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CP14

Infinite-Dimensional Black-Scholes Equation with Hereditary Structure

This paper considers the option pricing problem for contingent claims of the European type in a (B,S)-market in which the stock price and the asset in the riskless bank account both have hereditary structures. The Black-Scholes equation for the classical option pricing problem is generalized to an infinite-dimensional equation to include the effects of time delay in the evolution of the financial market as well as a general payoff function. It is shown that the pricing function is the unique viscosity solution of the infinite-dimensional Black-Scholes equation. A computational algorithm for the solution is also obtained via a double sequence of polynomials of a certain bounded linear functional on a Banach space and the time variable.

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CP14

A Comparison of Numerical Optimization Techniques for Financial Markets

We study mathematical models, dynamical systems, and numerical optimization techniques with parameter identification related to price dynamics. We implement the corresponding algorithms and compare their performance. We test the algorithms on a large set of closed end funds trading in US markets.

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CP14

A Condition Number for the Integral Representation of American Options

The pricing of an American option can be formulated as a free boundary value problem for the Black-Scholes equation. In this talk it is shown in which way the approximation error of the boundary influences the error in the option evaluation. A condition number κ depending only on the option parameters will be introduced to measure this deviation.

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CP14

Stochastic Models of Multimodal Systems of Cargo Delivery

A general scheme for modeling the transport flows interaction at trans-shipment points under uncertainty is presented. This scheme is based on the theory of semi-Markov and linear-Markov drift processes. The conditions are analyzed under which different types of interaction are most efficient: without warehousing, via warehouses,combined variant, etc. The boundary-value problems for systems of PDE are derived to determine the stationary joint distribution of queue-length of transport units and cargo at warehouse. Solving this problems is necessary step for determination of explicit expressions for items of total mean current expencies concerning transportation and trans-shipment of cargo. Reference: Postan, M.Ya. Economic-Mathematical Models of Multimodal Transport.Astroprint,Odessa,2006.

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CP15

Modeling Faculty Teaching Workload as a Linear Program

We present an assignment problem that distributes classes among instructors in the Mathematics department. Currently, the Director of Scheduling assigns about 190 classes to 60 instructors using the manual process of trial-and-error by considering, for example, an instructor's teaching workload and class preferences. However, this process is quite time-consuming. Therefore, we model the problem as a linear program with binary variables. Results are presented for the Fall 2006 schedule.

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CP15

A Special Class of Whispering-Gallery Modes in Billiards with Rational Caustics

Motivated by the search for optimized resonators of semi-conductor lasers one is interested in solutions of Helmholtz's equation for di-electrica analogous to whispering gallery solutions, but with the support localized in the interior of the resonator. By quasi-classical approximation solutions can be linked to classical trajectories in a mathematical billiard. In this talk it will be shown that billiards supporting a family of p-periodic orbits of the billiard map possess such solutions.

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CP15

Adaptive Radial Basis Function Methods with Residual Subsampling Technique for Interpolation and Collocation Problems.

We construct a new adaptive algorithm for radial basis functions (RBFs) method applied to interpolation, boundary-value, and initial-boundary-value problems with localized features. Nodes can be added and removed based on residuals evaluated at a finer point set. The shape parameters of RBFs are adapted based on the node spacings to prevent the conditioning growth of the interpolation matrix. Numerical examples in one and two space dimensions with nontrivial domains will be given.

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CP15

Mesoscopic Simulation of Self-Organization in Surface Processes

Self-organization of components of two phase mixtures through diffusion is known as Ostwald ripening. This multiscale phenomenon is well-suited to study using mesoscopic models which are stochastic partial differential equations that have been derived directly from the underlying microphysics. In this talk, spectral schemes for stochastic partial differential equations are described and verified using exactly solvable benchmark problems. These schemes are then applied to the mesoscopic model and the simulation results are compared with theoretical results such as the Lifshitz-Slyozov growth law.

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CP15

A Multigrid Approach to Spectral Methods for Time-Dependent Variable-Coefficient PDE

We present a high-order multigrid method for solving PDE of the form $u_t = Lu$. Coarse-grid correction is performed using Duhamel's Principle with the residual from the next finer level as the source term. At each level, a Krylov subspace spectral method is used to solve the appropriate PDE. Coarsening is achieved by performing canonical transformations in phase space, inspired by Fefferman's SAK Principle, to obtain approximate invariant subspaces corresponding to smaller eigenvalues of L.

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CP15

Mimetic Discretizations of Differential Forms and Operators

Compatible discretizations for solving partial differential equations are often used to preserve underlying physical properties expressed in the equations. Using algebraic topology, discrete differential complexes, and differential forms, it has been shown that mimetic methods (a class which includes examples of finite volume, finite element, and finite difference methods) can be placed in a common framework. This talk addresses existence and uniqueness of solutions to discrete div-curl systems that have been placed within this framework.

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CP16

Electromagnetic Scattering From an Anisotropic Impedance Half-Plane at Skew Incidence

A closed-form solution to the problem of scattering of an electromagnetic wave from an anisotropic impedance half-plane at skew incidence is presented. The governing equations reduce to a system of two first-order difference equations with periodic coefficients subject to a symmetry condition. The method leads toward a scalar Riemann-Hilbert problem on a hyperelliptic surface of genus 3. A procedure for this problem and also for the associated Jacobi inversion problem is proposed.

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CP16

The Timoshenko Model for a Compliant Offshore Structure

A system involving axial motion and beam displacement is considered for a compliant offshore structure model in an ocean environment. The response of the Timoshenko model is influenced by transverse loads, boundary conditions and a feedback action of the initial values of a steady-state response. Eigenfunctions of the beam model satisfy a damped matrix equation with non-commuting coefficients. Numerical experiments has been carried for Euler-Bernoulli, Rayleigh, Vlasov and Timoshenko beam models.

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CP16

Dynamic Matching in the TFT-LCD Cell Assembly Process

We consider the dynamic matching problem in the cell assembly process for producing TFT-LCD panel, where the mating of TFT array and Color Filter is assembled to produce a final product, the LCD display. The dynamic matching problem is formulated as a mathematical programming model, where the objective is to optimize the yield rate. In this new formulation, the precut layers are first grouped by different cut-types to reduce the modeling complexity. A yield matrix for the mating of two layers is then constructed. We explore the special structure of this new mathematical model; and new properties are established. Efficient algorithms are developed and computational performance of the developed procedures is investigated.

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CP16

Recurrence Relations for Regularized Coulomb Interactions and Application to a Treecode Algorithm

Recurrence relations are derived for the Taylor coefficients with respect to Cartesian coordinates of several regularized particle interactions, including the Coulomb potential, general power laws (e.g. Lennard-Jones), screened Coulomb potential (i.e. Debye-Huckel), and real space Ewald summation kernel. The recurrence relations are used in a particle-cluster treecode to accelerate the evaluation of potentials and long-range forces in molecular dynamics simulations. Results are presented for several cases including a time-dependent simulation of Newton's equations for a large number of particles.

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CP16

A Multilevel Preconditioner for FEM Modeling of Semiconductor Devices

Preliminary results for an unstructured mesh stabilized finite element formulation of the drift diffusion equations to model semiconductor devices will be presented. A parallel Newton-Krylov method is preconditioned by a multilevel method based on an aggressive coarsening algebraic method involving a graph partitioning algorithm. A brief motivation, overview of the formulation and preliminary results are presented. Performance results for domain decomposition and multilevel solution methods on large-scale simulations will also be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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CP16

Phononic Band Gaps with Effects of the Density Ratio and Contrast of Elastic Constants

We develop a fast method for computing band structures of phononic band gap materials with particular emphasis on the effects of the density ratio and of the contrast of elastic constants. First, we explore an omnidirectional reflector in a wide range of frequencies. Next, we consider two-dimensional arrays of different media embedded in rubber. Third, we examine the modes of waveguide that propagate along the cylinder axis of two-dimensional phononic band gap materials.

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CP17

Adaptive Panel Method for Particle Simulation of Three Dimensional Vortex Sheet Motion

New local, adaptive, higher order, tree-based quadrature and point insertion method to describe 3-D vortex sheet motion . This method for the first time enabled us to consider long time behavior of unstable vortex rings and rings collision. Not limited to vortex ring motion and can be applied to any vortex sheet such as jets and wakes. The topic is interdisciplinary including Applied Mathematics, Physics, Fluid Dynamics, as well as Computer Science (recursive tree-codes).

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CP17

Krylov Subspace Spectral Methods for Conservation Laws

Krylov subspace spectral methods have been shown to be effective high-order methods for solving variable-coefficient time-dependent scalar PDE. In this talk, we present a generalization to systems of PDE, along with new results concerning their stability. We then present a modification of these methods to make them conservative. Wavelets are used instead of trigonometric polynomials for trial functions, and it is shown that we can obtain highly accurate cell averages of the residual, which helps to enforce conservation.

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CP17

Granular Flows in Convering Hoppers: Inserts and Mass Flow Limits

Two models of granular flow through a converging nonaxisymmetric hopper are considered, for comparison to each other and to experimental results. The resulting first order nonlinear partial differential algebraic systems admit similarity solutions for stress, velocity, and a plasticity coefficient. A pseudospectral discretization is applied and the resulting solutions compared. The effect of inserts into the hopper is explored, as is the idea of computational determining the mass flow limit.

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CP17

Strictly Stable Wave Propagation in Discontinuous Media and Complex Geometries

Strictly stable approximations are derived for the second order wave equation in discontinuous media and complex geometries. The discontinuity is treated by splitting the domain at the discontinuities in a multi block fashion. Each sub domain is discretized with compact second derivative summation by parts operators, and the blocks are patched together to a global domain by using a penalty method. The analysis is verified by numerical simulations in two and three spatial dimensions.

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CP17

An Implicit, High Resolution Riemann Solver for Time Dependent Particle Transport

We present a Riemann solver for the spherical harmonics (P_n) approximation to the radiation transport equation. To make the high resolution scheme implicit in time, it is necessary to solve a system of nonlinear equations at each time step. This is accomplished using an two-step method that eliminates the need for a traditional nonlinear solver. Results are presented that show auspicious agreement with analytical solutions and other benchmarks using time steps well beyond the CFL limit.

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CP17

Stochastic Modeling of Traffic Flow

We employ a novel energy driven stochastic model in order to describe the complex traffic flow phases which arise for different concentration regimes. A major advantage of the proposed stochastic model is that it lends itself to analysis and, most importantly, no ad hoc noise is introduced. Kinetic Monte Carlo simulations are used to validate the proposed model against experimental data.

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CP18

Complex Hermite-Gaussian Approximation to the Mode-Locked Laser

We examine a new numerical discretization of the complex-valued governing equations of an actively mode-locked laser via a novel mapping. The resulting approximation is based on a set of shifted Hermite functions on an infinite line. Numerical comparisons are given with a finite difference scheme on a mapped domain as well as a finite element method on a truncated domain for various time stepping schemes.

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CP18

Mesh Redistribution in the Least-Squares Finite Element Methods

This work concerns optimal grids construction for solutions of convection dominated flow problems based on least squares finite element approximations. Redistribution approach is considered to generate the optimal grids. Numerical results which lead to an appropriate grading of optimal grids for weighted least squares finite element methods will be provided. Theoretical results on the choice of weighting functions will also be presented.

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CP18

A Method to Generate a Grid with Prescribed Volumes

We study methods of adaptive grid generation for given cell volumes in the two dimensional domain. We present two different methods, one is using the deformation theory, called deformation method and the other is our alternative approach, displacement method. Both techniques lead to qualitatively similar grid configurations. We further compare the numerical accuracy and CPU time of these two methods. We show that our displacement method has advantages in both CPU time and achieving desired accuracy.

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CP18

On the Solution of Heat-Like Equations by the Hy-

brid Laplace Transform/Finite Difference Method

The effect of spatial truncation errors on inverting the Laplace transform in the hybrid method for solving heat-like partial differential equations is examined. Using four characteristic problems, the accuracy of the hybrid method is compared against the exact and Crank-Nicolson solutions when the Fourier and a regularization method are used to invert the Laplace transform. It is shown that for sufficiently high spatial resolution both methods give excellent results.

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CP18
Domain Decomposition Applied to Biharmonic Problems

Steady-state 2-D creeping flow problems are governed by the biharmonic equation for the streamfunction. Classical solutions exist for simple geometries such as a wedge, sphere, and driven cavity. We present a method for developing numerical solutions in more complex geometries using a domain decomposition procedure solving a set of coupled equations. The procedure allows high-order accuracy, is computationally efficient, and provides a natural framework for local grid refinement. Several examples will be presented.

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CP19
Use of Fish Fin Rays for Hydrodynamic Efficiency

Fish fins have evolved over millions of years in a convergent fashion, leading to a highly-intricate fin-ray structure that is found in half of all fish species. This fin ray presumably arose for reasons of efficient hydrodynamic interaction. We will present a simple model of the fin ray, which identifies the key geometrical and mechanical parameters for performance. The model is optimized for mechanical advantage, leading to structures which resemble the natural structures. We will then present simulations of a fully-coupled fin-fluid model which helps us understand the efficiency of fish swimming through the phenomenon of vortex shedding.

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CP19
Vortex Sheet Simulations of 3D Boussinesq Flow Using a Treecode and Triangular Panel Method

We develop a method to compute vortex sheet motion in a Boussinesq three-dimensional flow. The sheet is represented as a set of Lagrangian particles lying on an adaptive triangular mesh. To resolve the severe stretching of the sheet, remeshing is performed after each time step. A panel method and tree code are used to evaluate the velocity. Computational results will be shown.

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CP19
A Moving Mesh Finite Element Method for Nonlinear Time-Dependent Pdes

The derivation and application of a new moving mesh finite element algorithm will be described for the solution of general families of time-dependent parabolic PDEs of second and fourth order. The mesh evolution is based upon ensuring local conservation of prescribed monitor functions as the solution evolves. Results will be presented and assessed for problems in one, two and three space dimensions.

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CP19
Synthesis of Force-Free Magnetic Fields Via Curl Operator Eigenvalue Problems with Non-Classical Boundary Conditions

Lorentz force minimization often constrains high intensity magnetic field device design. Force-free fields, with magnetic fields locally parallel to their curl, can arise as eigenfunctions of the curl operator. For smooth, topologically non-trivial domains, boundary conditions rendering the curl operator self-adjoint are non-local, and form an infinite dimensional space. The isotopy invariant subset however, is elegantly parameterized and, via Whitney forms, provides an effective tool for finite element discretization of the curl operators eigenvalue problem.

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CP20

Multilevel Methods for Dual Total Variation Minimization

This work describes a computational method for the inverse problem of edge-preserving image restoration. Total Variation (TV) regularization removes noise from an image while retaining its edges. Earlier primal TV methods require a user-chosen smoothing parameter which, if chosen too large, will lead to blurred edges . We solve an equivalent dual version of the TV problem independent of a smoothing parameter. Our multigrid methods show faster convergence than the Chan-Golub-Mulet primal-dual system of PDEs.

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CP20

Displacement Rank Concept for Solving the Inverse Problem of Electrical Impedance Tomography

Applying the conventional Output Least Squares method to the nonlinear inverse problem of Electrical Impedance Tomography involves the inversion of a sequence of dense nonstructured matrix problems. Given the dimensionality of currently studied 3D problems, such an approach becomes computationally prohibitive. Starting from a modified problem formulation which retains the underlying sparsity structure, we derived a fast iterative solution method based on imbedding the original displacement rank concept in a conjugate gradient scheme.

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CP20

A Posteriori Error Estimates for An Augmented Mixed Finite Element Method in Linear Elasticity

We develope an a posteriori error analysis for an augmented mixed finite element method for the problem of linear elasticity in the plane. We derive both residual and Bank-Weiser type a posterori error estimators for the case of mixed boundary conditions.

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CP20

Existence Theorem for Functional Differential Equations with Advance and Delay

Functional Differential Equations (FDEs) with advanced and delayed arguments arise in the nerve conduction theory, cell growth and several other applications. Here, we discuss various formulations of initial value problems associated with such FDEs and prove an existence theorem.

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CP20

Structure Preserving Solution Method for Electrical Impedance Tomography

The well-established concept of subspace algorithms has led us to introduce a new structured problem formulation for Electrical Impedance Tomography. Whereas conventional output-least squares methods can be regarded as minimizing a certain error norm, solutions are recovered here as the minimizers of a closely related residual norm problem. An iterative solution scheme is shown to lead to a sequence of structured sparse matrix problems, the conditioning of which appears to be far more favorable than typically observed in output least squares.

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CP21

A Novel Distribution Classifier

We present a novel classifier for a collection of densities. In information theory, capacity is the smallest radius enclosing these distributions, in terms of information divergence. Our problem is , given two sets of distributions, called normal data and abnormal data, to find a classifier with the smallest radius enclosing these normal data and, excluding abnormal data. Based on this, we propose a model to find such a classifier. We show the existence and uniqueness of the classifier theoretically, and suggest an efficient algorithm.

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CP21

Jammer Mitigation Via Space-Time Adaptive Processing

The use of the Global Positioning System (GPS) for accurate knowledge of geographical location and timing information has become ubiquitous. This paper concerns the mitigation of GPS receiver jamming. The focus is on the implementation of spacetime adaptive processing (STAP) algorithms to mitigate jamming. We illustrate the performance of STAP by analyzing the frequencyangle response (FAR). Explanations and visualizations of algorithmic performance, in terms of jammer mitigation and satellite availability, are provided for different jammer types and angular locations.

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CP21

A Network Analysis of Committees and Subcommittees in the United States House of Representatives

Network theory provides a powerful tool for the representation and analysis of complex systems of interacting agents. Here we investigate the networks of committee and subcommittee assignments in the United States House of Representatives from the 101st–108th Congresses, with committees connected according to interlocks" or common membership. We examine the House's community structure using several algorithms and reveal strong links between different committees as well as the intrinsic hierarchical structure within the House as a whole. We combine our network theory approach with analysis of roll call votes using singular value decomposition and successfully uncover political and organizational correlations between committees in the House without the need to incorporate other political information. This is joint work with Peter Mucha, Mark Newman, A.J. Friend, and Casey Warmbrand.

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CP21

Shape Scale: Representing Shapes at Their Absolute Scales

Scale space idea is used in many computational vision tasks including extraction of local symmetries. Despite its appeal, the idea has not been applicable in generic shape recognition. The selection of the same coarsening parameter for different shapes does not guarantee that these shapes will be represented at the same scale. Geometric shape may behave different than a self similar fractal and it may have its own absolute scale at which it has to be interpreted. We propose an alternative hierarchical representation in which each simple closed curve is represented at an absolute scale determined by its geometry and topology. Iterative diffusion is used as the basic implementation mechanism.

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CP22

A Posteriori Error Estimators for a Two-Level Finite Element Discretization of Viscoelastic Fluid Flow

We derive locally calculable a posteriori error estimators for a two-level method of discretizing the equations of steady-state flow of a viscoelastic fluid obeying an Oldroyd-type constitutive equation with no-slip boundary condition. The two-level algorithm consists of solving a small non-linear system of equations on the coarse mesh and then using that solution to solve a larger linear system on the fine mesh. Specifically, following Najib and Sandri, we use a Newton linearization on the Oldroyd-type constitutive equation about the coarse mesh solution thus nullifying the difficulties brought by the advection term. Our theoretical error estimates show that it has optimal order accuracy provided the true solution is smooth and its norm is sufficiently small. In addition, our computational error estimates exhibit the validity of our analysis.

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CP22

Resistive Oscillation in Planetary Magnetic Fields

Planetary magnetic fields, including the Earth's, are generated by dynamo action in fluid cores. These planetary cores are modeled as thin spherical shells containing an electrically conducting fluid. Asymptotic techniques are used to study slow oscillations with very short wave lengths. Possible instabilities for given ambient magnetic fields are of primary interest. Short wavelength solutions are important since most numerical dynamo models are unable to capture dynamo behavior at such length scales.

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CP22

Point-Scattering Description of Headwaves in An Acoustic Medium

In this talk we provide the point scattering description of headwaves for a simple acoustic medium with one interface. We start with the construction of solution for the three dimensional Helmholtz equation using the perturbative approach of scattering theory and analytically continue these solutions using Padé approximants. The approach allows the description of a point-source experiment including large offset arrivals and headwaves. An interesting representation of these solutions using Feynman diagrams will also be discussed.

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CP22

Analysis of Acoustic Influence of Frequency Variation in an Upper-Sediment Model

Acoustic propagation in sandy shallow-water environments

is modeled using a convenient parameterization to investigate influences of sediment frequency variations. The modal attenuation coefficients for isospeed-layer environments show a rapid decrease as frequency increases from 10 to 1000 Hz. However, the addition of a geoacoustic structure that models a thin poro-elastic sediment produces modal attenuation coefficients that increase with frequency. This behavior corresponds to experimental findings in the literature.

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CP22

Two-Component Miscible Displacement in Fractured Media

In this talk, we present a model which describes the effects of turbulent mechanical mixing of nonstationary, incompressible, two-component, miscible displacement in fractured media with moderate-sized matrix blocks. In a fractured medium, there is an interconnected system of fracture planes dividing the porous rock into a collection of matrix blocks. The fracture planes, while very thin, form paths of high permeability. Most of the fluids reside in matrix blocks, where they move very slow. Let ϵ denote the size ratio of the matrix blocks to the whole medium and let permeability, gravity and width ratios of matrix blocks to fracture planes be of the orders ϵ^2, ϵ and ϵ^0 respectively. Microscopic models for the two-component, miscible displacement in fractured media converge to a dual-porosity model as ϵ tends to 0. In this macroscopic model, domain is regarded as a porous medium consisting of two superimposed continua, a continuous fracture system and a discontinuous system of matrix blocks. The two-component miscible flow is formulated by conservation of mass principles for each continuum. Matrix blocks play the role of a global source distributed over the entire medium. A source term is included in flow equations in the fracture system, which representing the exchange of fluid between matrix blocks and the fractures.

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CP23

Dynamics of Density Stratified Vortex Sheets in an Inclined Channel

A model of two incompressible, immiscible density stratified fluids subject to Kelvin-Helmholtz instability is considered. The approach uses a boundary integral representation in which the fluid interface is represented as a free vortex sheet and the channel walls as bound vortex or source sheets. The dynamics of the interface is studied numerically using the vortex blob method. The goal is to simulate the flow in the inclined channel and compare the numerical results with the experimental results obtained by Thorpe [J. Fluid Mech. 46 (1971) 299–319]. Singularity formation in vortex sheets in the channel is also analyzed and the results are compared with the case of unbounded vortex sheets as well as with long-wave model. If time permits, the effect of electrical field will be discussed.

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CP23

Steady-States and Tip-Streaming of a Slender Bubble with Surfactant in Extensional Flow

Slender-body theory is used to investigate steady-states and time-dependent evolution of an inviscid axisymmetric bubble in extensional Stokes flow, when insoluble diffusion-free surfactant resides on the bubble surface. The steady states reveal ellipsoidal bubbles covered in surfactant and, at larger strain, solutions with a cylindrical surfactant-free central part and endpoint surfactant caps. A model for time-dependent evolution at still larger strain is described which exhibits elongating tip-streaming filaments.

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CP23

Models for the Tear Film During a Blink

Lubrication theory for model problems that approximate the tear film on the eye are developed and solved numerically. The models incorporate viscosity, capillarity, and surfactant transport. The blink is modeled by a moving end of the film, and its periodic motion will be studied. The one-dimensional equations are put onto a fixed domain via a mapping, and the resulting PDEs are solved via a method of lines. The results are very encouraging for some conditions that are observed in vivo.

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CP23

Vortex Dynamics and Outflow Conditions in Subsonic Simulations of Soap Film Flow

You can visualize vortex shedding in 2-d flow past objects using a fast flowing soap film. The usual simulations with INS fail to capture the salient feature of the problem: film thickness variations! We present an overset grid method for a new 2-d compressible soap film model which captures thickness variations and complex vortex dynamics. Numerical results illustrate new non-reflecting outflow conditions which are transparent to pressure pulses and transported vortices in a "subsonic" regime.

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CP23

On Puck Motion Down a Thin Film on an Inclined Plane

We investigate experimentally and theoretically the motion of a freely moving puck down an inclined plane along a thin, viscous Newtonian fluid. The evolution equations describe the balance of the normal and tangential forces and a net torque balance, are found on two different time scales. This balance requires an excess pressure near the leading edge of the puck, evidence of which has been observed experimentally. In the quasi-steady limit, self-similar solutions are found, where the puck gradually sinks into the fluid and rotates in a direction parallel to the plane. However, the appearance of this solution depends on the dynamics dictated by the fast-time solution, which includes linear and angular acceleration terms.

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CP23

A Front Tracking Algorithm with Surface Tension and Mass Diffusion

The chaotic mixing of two distinct fluids has been a challange for theory, simulation and experiment for several decades. The Rayleigh-Taylor instability is a basic special case in which the mixing is driven by a steady accelerating force between fluids of different densities. In this case, a long standing problem has been the disagreements between simulations and experiments. In the work presented here, simulated mixing rates of Rayleigh-Taylor instability for miscible fluids with physical mass diffusion are shown to agree with experiment; for immiscible fluids with physical values of surface tension the numerical data lies in the center of the experimental values; for miscible flow when the visocity is dominant and mass diffusion is neglectable, the simulation data with physical viscosity (no regard to the numerical viscosity) agrees with experiment. The simulations are based on an improved front tracking algorithm to control numerical surface tension and on improved physical modeling to allow physical values of mass diffusion or surface tension. In summary, we find significant dependence of the mixing rates on scale breaking phenomena.

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MS0

Networks and Mathematical Epidemiology

Mathematics has long been an important tool in infectious disease epidemiology. I will provide a brief overview of compartmental models, the dominant framework for modeling disease transmission, and then contact network epidemiology, a more powerful approach that applies bond percolation on random graphs to model the spread of infectious disease through heterogeneous populations. I will derive important epidemiological quantities using this approach and provide examples of its application to issues of public health.

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MS0

Towards an Effective Image Registration Method for 4D CT Lung Images

In collaboration with Guerrero et al from MD Anderson Cancer Center, we are developing a new method for accurate registration of 4D CT lung images which accounts for: (1) the compressible nature of the lungs, (2) noise in the images, (3) higher computational workload. In order to account for lung compressibility, the pixel displacement is assumed to obey the continuity (conservation of mass) equation. Second, the effects of noise are alleviated by applying the local-global approach of Weickert et al. to the conservation of mass setting. Third, the resulting large scale linear systems are solved using a parallelizable, preconditioned GMRES algorithm. Preliminary numerical results obtained from applying the new method to 2D synthetic images, as well as 2D lung CT images, are promising. Current research focuses on modifying and extending the 2D implementation for the full 4D problem.

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MS0

Highly Accurate Prediction of mRNA Polyadenylation Sites using a Support Vector Machine

Messenger RNA (mRNA) polyadenylation is the process that is responsible for the 3' end formation of most mRNAs in eukaryotic cells. Prediction of mRNA polyadenylation sites (poly(A) sites) can help identify genes and define gene boundaries. Previous algorithms achieved moderate success in poly(A) site prediction. Here we describe an algorithm for highly accurate prediction of poly(A) sites that uses the enhancing cis elements that were identified recently and the support vector machine.

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MS0

A Condition Estimate for Pseudo-Arclength Continuation

Numerical continuation is the process of solving nonlinear equations of the form $G(u, \lambda) = 0$ for various parameter values, λ. Pseudo-arclength continuation is a technique that no longer solves $G(u, \lambda) = 0$ directly, but solves a newly parameterized version $F(u(s), \lambda(s)) = 0$ where s is arclength. We present a new characterization for certain classes of points that leads to an upper bound on $\|F'^{-1}\|$. This bound is needed to guarantee the convergence of Newton's method.

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MS0

Shape Analysis Using Spherical Harmonic Transform Applied to Surface Conformal Mapping

We propose a new method for visually detecting shape signatures of simply connected surfaces, using spherical harmonic transform of an inverse conformal map. Using the transform, space-invariant shape descriptors are obtained and normalized against sample mean. Two-dimensional visualizations of shape descriptors provide a global multi-resolution shape signature of surfaces. In particular, our descriptors are useful for visual detection of global patterns and creation of digital atlases in medical applications.

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MS0

Canonical Correlation Analysis Applied to Chemical Shift Imaging Data for Cancer Diagnosis

The analysis of Chemical Shift Imaging (CSI) data can be used as a non-invasive diagnostic tool to detect and localize the presence of a tumor, and to classify its nature. Recently, a fast and robust tissue typing technique has been developed. It is based on Canonical Correlation Analysis (CCA), which represents the multivariate variant of ordinary correlation analysis. Extensive simulation and in vivo studies, carried out on prostate CSI data as well as on brain data, show that CCA is very accurate and efficient.

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MS0

Surface-Based Disparity Map Computation for 3D Reconstruction

The disparity computation between images is of much importance for real-time 3D reconstruction. For the case of a rectified pair of images, the disparity between them can be though of as a map with features aligned in the same horizontal lines, i.e. sharing the same vertical coordinate. Hence, the mapping only affects the horizontal position between the images and can be visualized as a 2D manifold in 3D space. The algorithm developed for this application uses a representation of an image based on a truncated triangular wavelet expansion, which is constrained to yield a conforming triangulation. This triangulation is also used for representing the disparity map which is computed over time as an update of previous estimates. As part of the algorithm, multiscale operators are defined in the triangulated domain for smoothing and convergence of an energy functional to determine the optimal disparity map.

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MS0

Image Partition Regularity of Affine Transformations

Let $u, v \in \mathbb{N}$, let A be a $u \times v$ matrix with rational entries, and let $\vec{b} \in \mathbb{Q}^u \setminus \{\vec{0}\}$. Let S be one of $\mathbb{N}$, $\mathbb{Z}$, or $\mathbb{Q}$. We say that the affine transformation $\vec{x} \mapsto A\vec{x}+\vec{b}$ is *image partition regular* over S provided that whenever S is partitioned into finitely many cells, one cell contains the image of $\vec{x}$ for some $\vec{x} \in \mathbb{Q}^v$. We determine precisely when A is image partition regular over $\mathbb{N}$, $\mathbb{Z}$, or $\mathbb{Q}$. We will also present the history of this problem.

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MS0

Adaptive Local Refinement

Local refinement enables us to concentrate computational resources in areas that need special attention, for example, near steep gradients and singularities. This talk will discuss a strategy for determining which elements to refine in order to optimize the accuracy/computational cost. Set in the context of a full multigrid algorithm, our strategy leads to a refinement pattern with nearly equal error on each element. Further refinement is essentially uniform, which allows for an efficient parallel implementation.

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MS0

Cost-Benefit Analysis of a Rotavirus Immunization Program in the Arab Republic of Egypt

Rotavirus diarrhea is a significant cause of morbidity and mortality in Egyptian children aged 0-5 years. In light of recent developments in rotavirus vaccine development and licensing, one contributing factor to assist decision and policy makers on whether to add rotavirus vaccination to national immunization programs is to understand the costs and benefits from such type of policy decision. In Egypt, approximately 1,799,000 children are born each year. Within this birth cohort of children, 3000 die before they reach the age of five, while close to 1,709,000 will have become ill with rotavirus by the age of five. The Egyptian Ministry of Health and Population (MoHP) is the main payer of health care and responsible for administering the Expanded Program on Immunization with the country. To inform these decision makers, a cost-benefit analysis, from the perspective of the MoHP, based on available local data from published and unpublished sources was conducted to evaluate the economic impact of introducing a rotavirus vaccine to the current national immunization schedule.

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MS0

Talk Title To Be Announced

Abstract not available at time of publication.

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MS0

Implementing High-performance Multigrid Software

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MS0

Basic Issues and Tools in Scientific Programming

Input your abstract, including TeX commands, here. The abstract should be no longer than 75 words. Only input the abstract text. Don't include title or author information here.

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MS0

Talk Title To Be Announced

Abstract not available at time of publication.

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MS1

Extracting s-wave Scattering Lengths from BEC Dynamics

At extremely low temperatures, elastic collisions between bosonic atoms are characterized by a single microscopic parameter: the atomic s-wave scattering length. This parameter also characterizes most of the macroscopic properties of a Bose-Einstein condensate (BEC). In a system of two BECs, three s-wave scattering lengths characterize the microscopic interatomic interactions (intra- and interspecies), as well as the macroscopic interactions between the two condensates. I will discuss a technique that attempts to extract the ratios of these scattering lengths by examining the macroscopic BEC dynamics that result from the sudden creation of a binary condensate in two spin states of ^{87}Rb. The experimentally observed atomic density distributions exhibit striking transient ring patterns that match closely the results of numerical simulation.

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MS1

Multi-Component Vortex Solutions in Coupled NLS Equations

A Hamiltonian system of coupled nonlinear Schrodinger (NLS) equations is considered in the context of experiments in photorefractive crystals and Bose-Einstein condensates. Due to the incoherent coupling, the Hamiltonian system has a large group of symmetries that include symmetries with respect to gauge transformations and polarization rotations. We show that the group of symmetries generates a large family of vortex solutions that include vortices with double charge and hidden charges. New families of vortices with different charges at the same component are also constructed and their stability problem is block-diagonalized to a simpler form, which is convenient for numerical analysis of unstable eigenvalues. In particular, we show that the hidden-charge vortex is less stable compared to the double-charge vortices under the presence of symmetries. Our results hold both for continuous and discrete versions of the NLS system. This is a joint work with A. Desyatnikov (Australian National University) and J. Yang (University of Vermont).

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MS1

Bose-Einstein Condensates in Optical Lattices and Superlattices

Bose-Einstein condensates (BECs), formed at extremely low temperatures when particles in a dilute gas of bosons condense into the ground state, have generated considerable excitement in the atomic physics community, as they provide a novel, experimentally-controllable regime of fundamental physics. In this talk, I will discuss my research on the macroscopic dynamics of coherent structures in BECs loaded into optical lattice and superlattice potentials, for which I employ methods from dynamical systems and perturbation theory. Using Hamiltonian perturbation theory, I will give an analytical construction of wavefunctions (observed in recently reported experiments) whose spatial periodicity is an integer multiple of the lattice period. I will also discuss BECs in superlattice potentials and how to manipulate solitary waves controllably with appropriate temporal adjustments of such potentials. Time permitting, I will briefly discuss more recent work on parametric excitation of BECs and work in progress on BECs with inhomogeneous (space-dependent) scattering lengths.

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MS1

Derivation of the Gross-Pitaevskii Equation for Rotating Bose Gases

The Gross-Pitaevskii equation is commonly used to describe dilute, trapped Bose gases at zero temperature. We present a proof of its correctness for the description of the ground state energy and corresponding one-particle density matrix of such systems with repulsive two-body interactions, starting from the underlying many-body Schrödinger equation. Our result applies to both rotating and non-rotating Bose gases. In particular, we prove the occurrence of complete Bose-Einstein condensation and superfluidity in the system. In the case of a rotating Bose gas in an axially symmetric trap, our results show that the appearance of quantized vortices causes spontaneous symmetry breaking in the ground state. This is joint work with Elliott Lieb.

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MS2

Formal Logic, Set Theory, and Data Flow in the Implementation of a Differentiable, High-Performance PDE Simulation Toolkit

Sandia's PDE optimization and simulation toolkit Sundance is based on a high-performance kernel for sparse in-place functional differentiation of symbolic weak forms. The preprocessing required for setting up optimal evaluation objects in this kernel can be compactly represented in terms of a family of operations acting on the sets of nonzero functional derivatives at each node in the graph of a problem's weak form. This representation facilitates the analysis of the preprocessing algorithms used, and furthermore translates directly into compact and comprehensible code.

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MS2

Using Discrete Structure to Optimize Variational Forms

I will present some new results on automatic determination of efficient algorithms for evaluating element matrices for finite element methods. In previous work, we have shown how to evaluate element stiffness matrix by contractions between "reference tensors" encoding information about the form and basis functions and "element tensors" encoding information about the geometry and coefficients. I will present a new technique for optimizing this process based on finite geometry and how it may be combined with complexity-reducing metrics.

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MS2

Discrete Topological Structures

Numerical methods for PDEs can benefit from a geometric framework based on the notions of a fiber bundle and a sheaf of sections of a bundle. Motivated by these ideas we develop a discrete topological framework based on the notion of a Sieve that facilitates computation and geometrical reasoning about PDEs in the discrete setting. Following the ideas of etale topology, a Sieve encodes the topology of an abstract space in terms of its coverings by progressively ”finer” pieces. Physical and geometric fields (e.g., mesh coordinates) over a Sieve acquire natural notions of restriction and cocycle that facilitate the local computation and assembly phases. An important guiding principle of this work is the need to find natural discrete expressions of geometric ideas. These expressions are suggested by the specific nature of the computational process rather than by a simple transfer continuous concepts to software. In particular, our framework naturally accomodates the distributed nature of numerical algorithms implemented for parallel computers. We present examples of the use of the framework in the PDE-based simulations of compressible gas flow, geophysical dynamics and ion channel dynamics.

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MS2
Symmetric Groups for Mesh Refinement

Abstract not available at time of publication.

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MS3
A Geometric Analysis of Traveling Waves in a Bioremediation Model

Bioremediation is promising technology for cleaning contaminated groundwater and soil. The traveling wave corresponds to a moving Biologically Active Zone, in which microorganisms consume both substrate (contaminant to be removed) and acceptor (added nutrient). Using geometric singular perturbation theory we construct the traveling wave and indicate how properties of the wave can be used to determine its spectral stability.

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MS3
The Periodic Modulational Instability and the Krein Sign

We consider the (linearized) stability of a standing wave solution to the nonlinear Schrodinger equation with a periodic potential. We give a general condition (nonperturbative) which guarantees the existence of a modulational, or long-wavelength, instability. In the case of weak nonlinearity this instability has a nice interpretation in terms of the ”effective mass” of a particle in the periodic potential. We also analyze some finite wavelength instabilities. The possible ways in which such instabilities can bifurcate from the real axis can be related to the Krein sign of the eigenvalues.

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MS3
The Evolution of Hot Spots in Optical Parametric Oscillators

We analyze the stability and dynamics of pulse solutions of the parametrically forced nonlinear Schroedinger equation when the pulses also drive a thermal gradient in the medium. Depending on their relative sign and position, the pulses and their “thermal aprons” are seen to merge to form new stably bound multi-bump solutions that are rendered amenable to analysis through a disparity in spatial decay scales.

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MS3
Algebraic Stability of Semi-Strong Interactions in the Gray-Scott System

Recent work of Kaper and Doelman constructs multi-pulse solutions of the Gray-Scott systems in which localized activator pulses interact semi-strongly through a delocalized inhibitor. We consider a scaling of the Gray-Scott system for which the delocalized inhibitor is weakly damped, with a linearization whose essential spectrum is asymptotically close to the origin. Employing a novel renormalization group approach, we replace the exact linearization with a large perturbation which is able to control the flow local to the multi-pulse, and show solutions of the full PDE approach at an O(1) algebraic rate into an asymptotically small neighborhood about the formal pulse dynamics.

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MS4
Inverse Problems in Transient Thermal Imaging for Nondestructive Testing

We discuss efficient algorithms for the recovery of defects—either surface corrosion or internal cracks and voids—in an otherwise homogeneous object, from input heat flux/surface temperature measurements. Of particular interest in our analysis is the optimal choice for the input heat flux and measurement strategy which maximizes image resolution and stability. Conclusions will be illustrated with computational examples. This is joint work with Lester Caudill.

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MS4

Recent Developments in the Elliptic Systems Method for Time Dependent Diffusion Tomography

The elliptic systems method in its earliest forms was a PDE based approach to solving inverse problems in time dependent diffusion tomography. The author and his colleagues have expanded and simplified this method and its applicability in many ways, including working with multiple source positions and both continuous wave and more generally frequency based data. This talk will be centered on recent work, generalizations and examples with improved numerical results for problems with restricted data (backscattered or transmitted) for parabolic problems. A new semiparametric approach to noise reduction will be introduced that has wide applicability to all of the above problems.

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MS4

Parameter Identification in a Parabolic System Modelling Chemotaxis

Chemotaxis is the process by which cells aggregate under the force of a chemical attractant. The cell and chemoattractant concentrations are governed by a coupled system of parabolic partial differential equations. We establish identifiability of the nonlinear chemotactic parameter. A least-squares approach with Tikhonov regularization is used to find the chemotactic parameter. Numerical results are presented.

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MS4

Determination of Unknown Isothermal Surfaces by Thermal Imaging: Stability Properties

In this talk I will discuss the stability issue for an inverse parabolic problem arising from nondestructive evaluation by thermal imaging. The model of the problem is the determination of an unknown portion of the boundary of a thermic conducting body by prescribing initial and boundary values of the temperature and by measuring the corresponding thermal flux on an accessible and known portion of the boundary. The unknown part of the boundary is assumed to be an isothermal surface. I will show that, even when the unknown part of the boundary is a priori known to be smooth, the data are as regular as possible and all possible measurements are taken into account, still the problem is exponentially ill-posed, that is logarithmic stability estimates are essentially optimal. Finally, I will present an essentially optimal stability estimate with a single measurement, under some a priori information on the unknown part of the boundary and minimal assumptions on the data, in particular on the thermal conductivity. This is a joint with Michele Di Cristo and Sergio Vessella.

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MS5

Discrete Concepts and Algorithms in PDE Constrained Optimization

We propose a tailored discrete concept for optimization problems with nonlinear pdes including control constraints and develop a new discrete concept in pde constrained optimization with state constraints. The key idea consists in conserving as much as possible the structure of the infinite-dimensional KKT (Karush-Kuhn-Tucker) system on the discrete level, and to appropriately mimic the functional analytic relations of the KKT system through suitably chosen Ansätze for the variables involved. For both cases we provide numerical analysis, including convergence proofs and adapted numerical algorithms. As a class of model problems we consider optimization with (nonlinear) elliptic and parabolic pdes. This allows to validate and compare the new concepts to be developed against existing approaches for the class of elliptic control problems.

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MS5

Robustness Issues in Model Validation of Complex Processes

Methods for parameter estimation and design of optimal experiments are the key methods for validation of models. The paper presents new effective algorithms for robust parameter estimation and design of robust optimal experiments in dynamic systems. Numerical results for real-life applications from chemical engineering, robotics and aerospace will be presented.

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MS5

Robust Optimization in Cancer Treatment Planning

There are various sources of uncertainty in radiotherapy treatment planning for cancer, e.g. in calculated radiation doses and in organ location. Failure to take account of this uncertainty can lead to underdosing of the tumor and failure of the treatment plan. We describe robust optimization formulations and efficient algorithms for solving them, including a sequential linear programming algorithm for second-order cone programming.

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MS5

Sparse Covariance Selection Via Robust Maximum Likelihood Estimation

We address a problem of covariance selection, where we seek a trade-off between a high likelihood against the number of non-zero elements in the inverse covariance matrix. We solve a maximum likelihood problem with a penalty term given by the sum of absolute values of the elements of the inverse covariance matrix, and allow for imposing bounds on the condition number of the solution. The problem is amenable to interior-point algorithms for convex optimization.

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MS6

Contact with Slip in Multi-Material Eulerian Calculations

Multi-material Eulerian and arbitrary Lagrangian-Eulerian methods were originally developed for solving hypervelocity impact problems, but they are attractive for solving a broad range of problems having large deformations, the evolution of new free surfaces, and chemical reactions. The contact, separation, and slip between two surfaces have traditionally been addressed by the mixture theory, however the accuracy of this approach is severely limited. To improve the accuracy, an extended finite element formulation is developed and example calculations are presented.

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MS6

Interface Reconstruction with the Moment Data

A new mass-conservative interface reconstruction method is presented. Unlike volume-of-fluid methods, which calculate the interface location from the volumes of the cell fractions occupied by different materials, the new algorithm localizes the interface based on both volumes and centroids of the cell fractions. The normal of the linear interface in each mixed cell is determined by fitting the centroid of the fraction behind to the reference centroid. This results in a second order accurate interface approximation, which is shown to be more accurate than the volume-of-fluid counterparts.

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MS6

Multi-material Interface Reconstruction using Particles and Power Diagrams

We present a new method for interface reconstruction in multi-material flow simulations. The method introduces particles into mixed cells and uses an an attraction-repulsion model to draw particles of the same material type together. The interface is then reconstructed from the particles using a weighted Voronoi diagram or Power Diagram. The new method eliminates the material order dependence of the interface topology commonly seen in VOF reconstruction of three or more materials in a cell.

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MS7

On the Uniqueness of the Finite Deformation, Inverse Hyperelastic Problem

In most elastic reconstructions performed to date the tissue is modeled as a linear elastic material undergoing infinitesimal deformations. These assumptions render the forward problem linear, thereby simplifying the analysis and the solution of the inverse elasticity problem as well. However, for large compressions in quasi-static elasticity imaging, the assumptions of infinitesimal deformations and a linear response may both be incorrect. For example recent experimental data indicates that breast tissue stiffens significantly with applied strain (by an order of magnitude with 20 percent overall strain). With this as motivation we consider an inverse problem wherein finite deformations are allowed and the tissue is modeled as having a non-linear stress strain relation within a hyperelastic framework. We consider this problem in two dimensions and provide estimates of the number of deformation fields required to evaluate unique distributions of material parameters.

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MS7

Shear Stiffness Imaging Using MR and Ultrasound Acquired Data

The goal is to image the shear wave speed in tissue with the purpose of identifying cancerous tumor inclusions. We develop two algorithms: one algorithm utilizes the positions of propagating wave fronts in tissue; the second employs variance controlled differentiation where the window size is adjusted according to SNR. We show results from both algorithms with measured data. We also exhibit improvements when viscoelastic effects are taken into account. Data is from Mathias Fink's group at ESPCI in Paris, from Richard Ehman's group at Mayo Clinic, and from Kevin Parker's group at the University of Rochester.

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MS7

Characterizing Soft Tissue Stiffness Using Impulsive Radiation Force: Exploring the Potential for Modulus Quantification

Acoustic radiation force provides focused, short (¡0.1 msec) mechanical excitations in tissue. Tissue displacement is monitored using ultrasonic correlation methods. 2D images are typically synthesized from multiple excitations to display displacement at a given time after excitation. Here, we present methods for generating more quantitative metrics of shear modulus by combining information obtained within the excitation region with shear-wave propagation information from outside the ROE. Simulation, phantom, and in vivo data sets will be presented.

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MS8

Playing the Game: What I Have Learned

This talk will focus on developing a research career while being a successful teacher. It will also address the joys and challenges that one has with work and family.

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MS8

Juggling Eggs

At times (most times!) managing to cope with the pulls and pushes of an academic career – research, teaching, and service – while balancing your personal life and maintaining your sanity seems like juggling 5 eggs at a time. At every stage, at least 3 are up in the air, and you are certain that in a moment, you will have to mop up the floor. But somehow, you keep on juggling and nothing drops. In this talk, I will share my experiences in the tenure track, talk about my career in juggling, and describe my mistakes so you won't repeat them.

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MS8

Smooth Transitions and Turbulence: Shifts Between Professor and Administrator

Shifting into positions which require more administrative responsibilities can leave you wondering if your research has been lost in the transition. I'll speak about my experiences as a Director of Graduate Studies and as a Program Director at NSF and the challenges of keeping all the balls in the air.

Mary Ann Horn
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MS8

Developing a Commonsensical Approach to Academic Career

That other people's experience is relevant to yours, let alone that one can learn from it, is a questionable premise. With this caveat in mind, I will share some thoughts on surviving one's career choices, one step at the time.

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MS9

Nonholonomic Distribution and Utility Theory

Utility theory is one of the cornerstones of the modern economic theory. One of the critical aspects of the revealed preference relation is its rationality, e.g. absence of cycles, where each consecutive option is referable to its predecessor. We address here the question of existence of N-cycles in a preference relation. Its continuous relaxation leads naturally to a hyperplane distribution, which is nonrational if distribution is non-holonomic. We show that in each continuously non-rational preference relation there exists a finite cycle, and address the question of minimal length of such a cycle.

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MS9

Exterior Differential Systems and Billiards

Abstract not available at time of publication.

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MS9

Periodic Orbits in Outer Billiards

It is conjectured that in classical billiards periodic orbits constitute a set of zero measure and so far it is proved only for orbits of period 2 and 3. Recently, Genin and Tabachnikov proved that 3-period orbits in outer billiards have an empty interior. We prove that 4-period orbits in outer billiards also have an empty interior.

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MS9

Continuous Families of Periodic Orbits Via Control Theory

In this talk a control theory approach is used to construct classical billiards (different from elliptic domains) which possess continuous family of periodic orbits.

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MS10

Open Discussion

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MS10

Industrys Need for Computational Scientists and Engineers

Computation plays ever increasing and vital role in industry in many scientific areas; from modeling of gas turbines for jet engines to decrease testing to biological models for heart disease to speed clinical trials. In industry, there is an increasing reliance on computational models and simulations. To emphasize this, I will briefly describe a few examples of industrys trend toward simulation and modeling. As this trend continues, industry will continue to seek individuals with a computational science and engineering background. I will briefly describe what industry might be looking for when seeking to hire an individual with a computational science and engineering background. In closing, I will try to briefly describe how industry works and how to have an impact there.

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MS10

Internships and Work Experience in Undergraduate CSE Education

An internship or work experience can be the climax of a CSE undergraduate's education. With exposure to many new ideas, techniques, and applications at another institution, such an experience can greatly broaden and deepen the student's understanding of computational science and make the classroom education more meaningful. Moreover, work with a professional computational science team and contacts made during the summer can greatly enhance opportunities and options available to the CSE undergraduate.

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MS10

Introduction to the Report on Undergraduate CSE

This presentation will provide an overview of the report on Undergraduate CSE Education and an introduction to the contributors to both the report and the minisymposium. We will begin with our working definition of CSE, outline the sections and the topics for the presentations to follow. Attention will be paid to the differing forms and needs an undergraduate education in CSE can take and must try to meet.

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MS10

Undergraduate CSE Programs

The presentation will outline the major characteristics of the various types of undergraduate CS&E programs in the U.S. (i.e., minors, specialized majors, concentrations, certificates, etc). Specific examples will be presented. The talk will raise a number of questions for open discussion with participants: i) what are the "ingredients" for an undergraduate CS&E degree? ii) Major or minor or certificate? Pros and Cons; iii) what should be the learning outcomes of an undergraduate CS&E degree?

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MS11

Thyra and Rythmos: Object-Oriented Generic Programming for the Development of Transient Sensitivity Computations

Work is underway to develop a new library called Rythmos for transient simulation and sensitivity computations. Rythmos is being designed from the ground up to support algorithmic research into various types of transient simulation and sensitivity methods. Rythmos is being built on the foundation of Thyra for abstract vectors, vector spaces, linear operators, linear solvers, nonlinear solvers, and access to ODE/DAE models. The rational for Rythmos and the foundations of Thyra will be described.

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MS11

Nonlinear Full Approximation Multigrid for PDE-constrained Optimization

Large scale optimization of systems governed by partial differential equations (PDEs) is a frontier problem in scientific computation. In practice, one is rarely content with performing a simulation of a physical or engineered system; sensitivity analysis, parameter estimation, and optimization are required for a complete analysis and to reflect design goals. Instead of traditional trial-and-error approaches, optimization techniques that are efficient for large-scale systems have been devised, and their use results in orders-of-magnitude savings over traditional methods. In my talk I will describe a family of multilevel methods that exhibit parallel and algorithmic scalability. The main component is nonlinear full approximation scheme. The main questions are whether a full or reduced space are appropriate, what are the appropriate smoothing schemes, and what are the appropriate restriction and prolongation operators. I will discuss examples for problems with elliptic, and parabolic constraints.

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MS11

Automatic Differentiation and Large-Scale Optimization

Abstract not available at time of publication.

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MS11

Sensitivity Analysis for Systems Described by ODEs and DAEs

Derivatives with respect to problem parameters of solution components and/or functionals of the solution of dynamical systems are a critical ingredient for derivative-based dynamically-constrained optimization (as well as for many other types of analyses, such as model reduction, uncertainty quantification, etc). Obtaining such derivatives is the object of (local) sensitivity analysis (SA). We briefly overview the two possible approaches to SA for systems described by ODEs and/or DAEs, namely the forward and adjoint methods, and present the SA capabilities of the time integrators in the SUNDIALS suite.

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MS12

Magnetic Resonance Elastography: Introduction and Potential Medical Applications

A medical imaging technology capable of depicting the mechanical properties of tissue would be of great value, particularly for detecting cancer. The goal of our research is to develop MRI-based elastography methods, using novel techniques for visualizing propagating acoustic shear waves. Mathematical inversion algorithms are needed to process the acquired data to calculate tissue properties such as stiffness, viscosity, and anisotropy. Preliminary studies indicate that the technique has substantial potential as a diagnostic tool.

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MS12

Multiphase Mathematical Models for the Mechanics of Vascularized soft Tissue

Elastography techniques enable the quantitative measurement of tissue strain in vivo. An inverse problem to find the tissue biomechanical properties results, given the tissue's constitutive equation and the law of conservation of momentum. Typically tissue is assumed to be elastic or viscoelastic. However, soft tissues contain both fluid and solid phases. In this talk, we review and discuss mathematical models for multiphase mechanics and the resulting coupling between the fluid and elastic responses.

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MS12

Physical Bases of Elastography

Elastography methods are based on solving an inverse problem: determining unknown causes based on the observation of their effects. Ultrasound and MRI Elastography translate measured changes in the strain pattern in the tissue under various types of loading into a map of elastic properties of tissue. Another elastographic technique termed Mechanical Imaging is based on measurements of stress pattern to evaluate 3-D distribution of tissue elasticity. An overview of physical bases of various elastographic techniques will be presented.

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MS12

Dynamic MR/US Elastography as a Non-invasive Imaging Modality: In-vivo Application to Breast, Liver and Brain

Dynamic elastography offers the ability to measure the complex shear modulus at various frequencies. This can either be done in the transient or the stationary regime of wave propagation with MRI or Ultrasound. Each technique offers unique opportunities for certain aspects of elastography and certain applications. Results for breast cancer and liver fibrosis are presented. Initial results for in-vivo brain elastography are shown. Elastography as a tool to understand the rheology of tissue is discussed.

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MS13

On Balanced Truncation by Krylov Projection

Balanced truncation is one of the most powerful methods for model reduction. This method is similar to matrix approximation using the SVD. An open questions is whether balanced truncation can be accomplished by Krylov projection, that is interpolation methods. In this talk we will present results which establish such connection in a special case. This leads to approximate balanced truncation by rational interpolation.

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MS13

Inexact Krylov Projection Methods for Model Reduction

Rational Krylov subspaces are often capable of providing nearly optimal approximating subspaces for model reduction, although large linear systems of equations must be solved to generate the required bases. In practice, iterative solvers become necessary and choice of termination criteria and effect of preconditioning influences the quality of final reduced order models. General bounds on the H_∞ error associated with a reduced order model are introduced that provide a new tool to understand both features.

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MS13

An Iterative SVD-Krylov Based Method for Model Reduction

We propose a model reduction algorithm which combines the SVD and Krylov-based techniques.It is a two-sided projection method where the SVD-side depends on the observability gramian, and the Krylov-side is obtained via iterative rational Krylov steps. The reduced model is asymptotically stable, matches moments at the mirror Ritz values and is the best H_2 approximation among all reduced models having the same reduced system poles. Numerical results prove the effectiveness of the proposed approach.

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MS13

The Role of Sampling and Projection in Model Reduction

In this talk we show that several seemingly projection-based model reduction strategies do not require explicit system representation, but only a finite set of output frequency responses. Uncovering methods for which input-output frequency samples is sufficient is important, because such methods can easily be extended. As a demonstration, some of the sampling methods will be applied to example systems described directly by PDE's and by delay-differential equations.

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MS14

An Analysis of Partitioned Nonlinear Systems

In many application contexts, one can choose between various equivalent differential or integral equation models that in turn suggest discretization schemes and preconditioners for iterative methods for the solution of the corresponding discrete systems of equations. Effective preconditioners frequently use properties of the original continuous operators involved. I will present some recent work exploring iterations for solving nonlinear equations that arise from discretizing PDEs, specifically aimed at identifying criteria for distinguishing competing formulations.

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MS14

Maintaining the Non-Negativity of Numerical Solutions of Time-Dependent Reaction-Diffusion Problem

The solution to many application models should remain non-negative at all times for physical reasons. For a system of time-dependent reaction-diffusion equations as example, whose true solution is guaranteed to be non-negative, we discuss how non-negativity can be compromised in real-life calculations by the spatial discretization, the time discretization, the non-linear solver, and the linear solver. For the same example, we will show one way to enforce non-negativity of the solution numerically.

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MS14

Solving Hyperbolic PDEs in MATLAB

We have developed software in the MATLAB problem solving environment (PSE) that solves initial-boundary value problems for first order systems of hyperbolic PDEs in one space variable x and time t. Four explicit, central difference schemes are available in variants advantageous in the PSE. We have devised a convenient way to deal with rather general boundary conditions. Vectorization is key to the efficient implementation of the methods in Matlab.

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MS14
Solving PDEs with the VODE_F90 ODE Solver

We illustrate the use of a Fortran 90 extension, VODE F90, of the VODE ODE solver. Using PDE/MOL problems from chemical kinetics, polymer formation, and fluid flow, we illustrate new features including dynamic storage management, keyword options, root finding, solution constraints, and sparse Jacobians. We further illustrate the use of a MATLAB-like gui interface that simplifies specification of problem information, allows automatic generation of necessary subroutines, and provides convenient graphics.

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MS15
A Stochastic Immersed Boundary Method Incroporating Thermal Fluctuations: Toward Modeling Cell Micromechanics

The mechanics of many cellular systems involve elastic structures which interact with a fluid, for example the outer cell membrane deforms during protrusions generated during motility and cell organelles such as the Golgi Apparatus and Mitochondria involve membranes which deform and bud vesicular and tubular structures during biological processes. Modeling, analyzing, and simulating the mechanics of such systems presents many mathematical challenges. The immersed boundary method is one modeling approach for such systems, and has been applied to many macroscopic biological problems, such as blood flow in the heart and lift generation in insect flight. At the length scales of cells and cell organelles, thermal fluctuations also become significant and must be taken into account. In this talk we discuss an extension of the immersed boundary method framework which incorporates thermal fluctuations through appropriate stochastic forcing terms in the fluid equations. This gives a system of stiff SPDE's for which standard numerical approaches perform poorly. We discuss a novel stochastic numerical method which exploits stochastic calculus to handle stiff features of the equations. We further show how this numerical method can be applied in practice to model the basic microscopic mechanics of polymers, polymer knots, membrane sheets, and vesicles. We also discuss preliminary work on modeling the dynamics of cell organelle structures.

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MS15
Two Dimensional Movement of Nematode Sperm Cell

In this talk, I shall present numerical simulations of a two-dimensional moving boundary problem (MBP). Under appropriate conditions, this MBP possesses a traveling domain solution. We shall show that computationally, solutions of the MBP converge to the traveling domain solution as time goes to infinity for different types of initial domains. This MBP is an attempt to generalize the 1D model of Mogilner and Verzi (J. Stat. Physics, 2003) on crawling nematode sperm cell to 2D. The computation was done using level set method. If time allows, I shall outline the proof of the existence of traveling domain solutions.

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MS15
Mechanics of Bacterial Flagella

Bacterial flagellar filaments can abruptly change shape in response to mechanical load or changes in solution pH or ionic strength. These polymorphic transformations are an instance of a ubiquitous phenomenon, the spread of conformational change in large macromolecular assemblies. We propose a new theory for polymorphism, whose essential elements are two molecular switches and an elastic mismatch strain between the inner and outer cores of the filament. We calculate the phase diagram for helical and straight states, the response of a helical filament to an external moment, and discuss the effects of external flow.

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MS15
The Torque-Speed Relationship of the Bacterial Flagellar Motor

Many swimming bacteria are propelled by flagellar filaments driven by a rotary motor. Each of these tiny motors can generate an impressive torque. The motor torque vs. speed relationship is considered one of the most important measurable characteristics of the motor and so is a major criterion for judging models proposed for the working mechanism. With a previously developed efficient numerical technique for solving coupled Fokker-Planck equations (Xing, et. al., Biophysical Journal, 89: 1551-1563 (2005)), we give an explicit explanation for this torque-speed curve. The same physics can also explain certain puzzling properties of other motors. The work was published at PNAS 103: 1260-1265.

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MS16
Optical Manipulation of Matter Waves

Recent experimental and theoretical progress in the studies of Bose-Einstein condensation (BEC) has precipitated an intense effort to understand and control interactions of nonlinear matter-waves. Key ingredients in manipulations of matter-waves in BECs are a) external localized impurities (generated by focused laser beams) and b) periodic potentials (generated by interference patterns from multiple laser beams illuminating the condensate). In this talk we highlight the ability of time-dependent external optical potentials to drag, capture and pin a wide range of localized BEC states, such as dark and bright solitons. The stability and existence of pinned states is analyzed using perturbation techniques, which predict results that are well corroborated by direct numerical simulations. The control of these macroscopic quantum states has important applications in the realm of quantum storage and processing of information, with potential implications for the design of quantum computers.

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MS16

Soliton Dynamics and Scattering for the Gross-Pitaevskii Equation

We describe some results on long-time dynamics in Gross-Pitaevskii (or NLS) equations. We consider, in particular, classical soliton dynamics, and the nonlinear scattering problem.

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MS16

Topological Effects with Matter Waves: A New Twist on BEC

Ultracold gases present new opportunities to control and influence matter waves by clever manipulation of the trapping potential. For example, one can create beautifully ordered vortex lattices in a Bose-Einstein condensate by magnetic or optical "stirring" of the superfluid. In our laboratory at Georgia Tech we have used Bragg scattering to study these lattices, and have focused on the spatial profile of the diffracted atoms, which offers a new window into condensate physics. In addition to the mechanical forces, magnetic fields can also profoundly affect the wavefunction "simply" by coupling to the spin. We present a novel experimental realization of this coupling (and its rather dramatic consequences) using an "optically plugged" quadrupole trap (OPT) for sodium BECs.

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MS16

High Temperature Superfluidity and the Superfluid - Mott Insulator Transition in Ultracold Atomic Gases

Ultracold atomic gases are ideally suited to study strongly correlated many body systems. They provide clean, easy to model systems, where interactions can be tuned over an enormous range. I will discuss two recent experiments on high temperature superfluidity in a strongly interacting Fermi gas and the Superfluid - Mott Insulator transition of a Bose-Einstein-Condensate in a 3D optical lattice.

Christian Schunck
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sch

MS17

Modelling and Simulation of a Schistosomiasis Infection With Biological Control

A mathematical model is developed for a schistosomiasis infection that involves humans and intermediate snail hosts as well as an additional mammalian host and a competitor snail species. The model consists of a system of eight differential equations for the infected and susceptible subpopulations. The deterministic system is generalized to a stochastic system of differential equations to account for the random behavior of demographic changes in the population levels. Values for the parameters in the model are estimated and the populations are computationally simulated under various conditions. Results of the simulations indicate several interesting features such as the rapidity by which an invading competing snail species can change the dynamics of a schistosomiasis infection.

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MS17

SIS Epidemic Models with Multiple Pathogen Strains

The dynamics of discrete-time and continuous-time SIS epidemic models with multiple pathogen strains are studied. The population infected with these strains may be confined to one geographic region or patch or may disperse between two patches. The persistence and extinction dynamics of multiple pathogens strains in a single patch and in two patches are investigated. It is shown for the single patch model that the basic reproduction number determines which strain dominates and persists. The strain with the largest basic reproduction number is the one that persists and outcompetes all other strains provided its magnitude is greater than one. However, in the two-patch epidemic model, both the dispersal probabilities and the basic reproduction numbers for each strain determine whether a strain persists. With two patches, there is a greater chance that more than one strain will coexist. Analytical results are complemented with numerical simulations to illustrate both competitive exclusion and coexistence of pathogens strains within the host population.

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MS17

Asssessing Strategies for Control of Vector Borne Diseases

The control of vector-borne diseases is in many ways a different problem than the control of diseases that spread through person to person contact. Since the pioneering work of Ross in the late 19th and early 20th centuries, one classical approach for controlling vector-borne diseases involves the eradication or strict population control of the vectors. Vaccination, or other methods for generating resistance to the pathogen in humans, can also be effective, but since many vector borne diseases have a non-human amplifying host (eg. birds in the case of West Nile Virus) vaccination, even when a vaccine exists, is often less successful in controlling outbreaks than for a disease that is transmitted directly between human hosts. Furthermore, for many vector-borne diseases, there does not yet exist long term immunization measures for the hosts. Other options consist in prophylactic measures preventing contacts between vectors and hosts. Recent technological developments have made possible a potential new form of control, the genetic modification of vector species to introduce pathogen resistance. This presentation will examine the efficacy of different forms of control for a vector-borne disease through a mathematical model. We will introduce a model for transgenic control in the case of malaria, and investigate its potential utility.

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MS17

Estimation of the Reproductive Number and the Effects of Hypothetical Interventions During the Great Influenza Pandemic of 1918 in Geneva, Switzerland

I will present an analysis of historical hospital notification data of the 1918 influenza pandemic in Geneva, Switzerland. We estimated the number of secondary cases generated by a primary case during its period of infectiousness during the first two waves of infection. We then used these estimates to evaluate the single and combined effect of reductions in the overall influenza transmission rate via effective isolation strategies in hospitals or via reductions in the susceptibility of the general population through, for example, increasing hygiene and protective measures (e.g., increase hand washing, use of face masks), prophylactic antiviral use, and vaccination.

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MS18

Mechanical and Geometrical Aspects of Uterine Contractions

Uterine contractions play a critical role in labor and parturition and are an important factor in female reproductive health. However, how uterine contractions are regulated and controlled is not well understood. I analyze how structural components such as muscle layer arrangement and muscle wall geometry affect uterine contractions, utilizing a theoretical framework that makes the force-balance assumption of quasi-static equilibrium. Linear elasticity equations of passive deformation are also considered in order to investigate both non-pregnant and pregnant cases. Numerical analysis indicates that the existent muscle layer is necessary to achieve wall movement in the non-pregnant uterus with realistic forces as well as to minimize movement outside of the uterus organ. Model results indicate that a cylinder is a reasonable approximation to the uterus in the non-pregnant state. Other simulations indicate that the ellipsoid is likely a better approximation than the sphere to the term pregnant uterus. I discuss biological implications of these results and propose future extensions to the work presented.

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MS18

Sensitivity of Dynamical Systems to Banach Space Parameters

We study the sensitivity equations of general nonlinear dynamical systems in a Banach space with dependence on parameters in a second Banach space. First, we present an abstract theoretical framework for sensitivity equations and the numerical schemes to approximate the sensitivity equations. Then, we illustrate the theoretical results and the numerical methods with an application to measure dependent delay differential systems arising in a class of HIV models.

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MS18

Model Development and Evaluation for Trichloroethylene Metabolism in Humans

Trichloroethylene (TCE) is an industrial chemical and an environmental contaminant. TCE and its metabolites may be carcinogenic and affect human health. Physiologically based pharmacokinetic (PBPK) models that differ in compartmentalization are developed for TCE metabolism, and the focus of this investigation is on evaluating alternative models. Specifically, the model structures are compared through sensitivity analyses in order to discern what is necessary and what can be ignored computationally. (This abstract does not reflect EPA policy.)

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MS18

Superquadric Modeling in Computed Tomography Simulation

A novel asymptotic framework is presented to describe hydraulic fracture propagation. The problem consists of a system of nonlinear integro-differential equations, with local and nonlocal effects. This causes transitions on a small scale near the fracture tip, which control the behavior across the whole profile. These transitions depend upon dominant physical process(es), and are identified by simultaneously scaling the associated parameters with the distance from the tip. An analytic solution incorporating several processes is obtained.

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MS19

Hierarchical Approach to Design Optimization of Mechanical Systems with Multiple Frictional Contacts

We consider the design of mechanisms involving rigid body dynamics and multiple frictional contacts. Automated design of such mechanisms often requires numerical exploration of high-dimensional parameter spaces. Since exploration of this design space depends on accurate simulations of systems with many contacts that are intermittent, frictional, and locally compliant, a naive search can be infeasible for even simple systems. Verification with the dynamic model adds even more complexity to the problem as some region of dynamic model parameters must be sufficiently sampled for each point in design space. We are describing a hierarchical method for design optimization that relies on reduced-order models to efficiently prune both the design and model spaces, that are refined to explore and optimize feasible designs. We illustrate the results with simulations and experimental prototypes.

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MS19

Semicopositive Linear Complementarity Systems

After reviewing existing well-posedness results of linear complementarity systems (LCSs), we present new results on the existence and uniqueness of weak solutions to LCSs with strictly semicopositive matrices, whose definitions in an integral form are shown to be equivalent to a well-known vector-matrix definition. The existence is based on a constructive time-stepping scheme, and the uniqueness on an explicit connection to Mandelbaum's dynamic complementarity problem and on the integral form of strict semicopositivity.

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MS19

Dynamical Systems Subject to State-induced Mode Changes

In various applied domains, such as friction mechanics, power converters, and resource networks, one finds systems that are subject to internally induced abrupt changes of behavior. The modeling framework of *cone complementarity systems* applies in this context. Well-posedness issues lead to the consideration of linear complementarity problems that are in some cases nonstandard in the sense that both globalness and uniqueness of solvability are only required in a qualified sense.

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MS19

Convolution Complementarity Problems and Impact Mechanics

Convolution complementarity problems (CCP's) are a kind of dynamic complementarity problem of the form $0 \leq u(t) \quad \perp (k * u)(t) + q(t) \geq 0$ for all t. These generalize the Linear Complementarity Systems of Schumacher et al. in the sense that k need not come from a matrix exponential. Some complementarity problems with PDE's lead to systems of this kind with $k(t) \sim K_0 t^{\alpha-1}$ for small t with $0 < \alpha < 2$ and K_0 s.p.d. We will see how this affects existence and uniqueness questions for CCP's, and what this means for applications such as impact problems.

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MS20

Microscopic-macrosopic Characterization of Viscoelastic Materials

The classical characterization tools of viscoelastic materials are "macroscopic". Devices impose either a stress or deformation boundary condition, at sufficiently low levels that the material response is in the linear regime, and either deformation or stress is measured to infer the material properties. It has always been of interest to develop experiments and associated theory that allows one to characterize materials in the nonlinear regime, typically involving heterogeneous flow or deformations and associated viscoelastic stress features. In the past decade, there has been an upsurge in microscopic characterization tools and models, with advanced instrumentation and new modeling challenges. The key modeling advances require a sophisticated understanding of stochastic and deterministic behavior of small probe particles in viscoelastic media, or of ensembles of small particles of various shapes and degrees of rigidity in viscous solvents. This minisymposium highlights several advances, ranging mathematically from computational to applied analysis to new rigorous analysis, and scientifically from instrumentational advances to new features of complex biological systems.

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MS20

Beads in Mucus, Generalized Langevin Equations, and State Space Models

High speed microscopy has enabled experimentalists to track individual microbeads in complex fluids such as human lung mucus. The dynamics of such a bead in a viscoelastic fluid is governed by the generalized Langevin equations. In this talk, a maximum likelihood method to estimate parameters for a certain class of generalized Langevin equations will be presented. In addition, an improved stochastic simulation method for this class of models will be shown.

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MS20

Computational Studies of Nematic Liquid Crystalline Polymers in Planar Shear Flow

We present fully three-dimensional numerical simulations of the dynamics of the Doi-Marrucci-Greco model for nematic liquid crystals. The model couples the Smoluchowski equation for the orientational distribution function with the Navier-Stokes equations, via a closure approximation. The simulations show the formation and dynamics of roll cells and disclinations, and are in both qualitative and quantitative agreement with recent experiments.

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MS20

Mesoscopic Structure Phenomena in Sheared Rigid Rod Dispersions

I will present recent analytical results on 2-D nematic polymers under weak shear.

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MS21

Optimal Experimental Design in Molecular Life Sciences

The Systems Biology Markup Language has been established as a standard XML notation for models of biological systems. Two main reasons impede the direct application of existing tools for optimal experimental design from the field of model-based engineering. First, they cannot derive a DAE system from an SBML description. Second, they are unable to reflect variety of experimental set-ups. We present a very effective tool that overcome these limitations and results for real-life applications.

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MS21

Optimizing Control of Reactive SMB Processes

Simulated Moving Bed processes are difficult to control due to their hybrid dynamics, spatially distributed state variables with steep slopes, and slow and strongly nonlinear responses of the concentration profiles to changes of the operating parameters. This contribution deals with the optimization-based control of reactive SMB processes where the operating parameters are optimized over a finite horizon to minimize an economic cost function while the product purities appear as constraints in the optimization problem.

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MS21

Issues in the Practical Implementation of Near Time-Optimal Control of Robots

Making robots perform repetitive tasks faster has benefits in increased manufacturing productivity. There is a very substantial gap between numerical solution of time-optimal robot maneuvers, and implementing such fast maneuvers routinely in hardware. This paper summarizes results that aim to fill this gap, including handling of vibrations, making use of existing controllers, supplying optimized nonlinear feedback with NMPC, and conversion to regulation at the end of the maneuver.

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MS21

Detailed Numerical Simulation of Reactive Flows in Catalytic Channels

Using the boundary-layer assumption, the steady-state laminar flow through a catalytic channel is simulated numerically. The chemical processes are modeled by elementary-step kinetics involving intermediate species in gas-phase and on the surface. Furthermore, the transport coefficients are derived from molecular data for each species mixture. The large and stiff DAE systems are solved by a new code, based on backward differentiation formulas. Direct shooting is then used to solve an optimal control problem.

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MS22

Optimal Nodes for Radial Basis Function Interpolation

Radial basis functions (RBFs) provide mesh-free approximations suitable for interpolation and the solution of differential equations. Like polynomials, RBFs can be spectrally accurate but suffer from potential instabilities such as the Runge effect. In a special case, Gaussian RBFs can be transformed to polynomials and thus studied using potential theory. From this one can find node distributions that are stable for all functions analytic on the interval of approximation.

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MS22

Point-to-point and Volumetric Measures of Uniformity of Point Sets

Abstract not available at time of publication.

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MS22

Optimal Points for High Dimensional Problems

For numerical integration, numerical function approximation, and statistical design of experiments, the positioning of the sample points, also called the design, influences the error of the approximation. Several measures of design quality appear in the literature, such as, fill distance, separation distance, discrepancy, and energy. Designs that optimize these different quality measures may or may not look the same. This talk reviews these different quality measures, explains the connections between them, and demonstrates their role in error bounds.

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MS22

Maximum Area with New Measures of Perimeter

The oldest competition for an optimal shape (area-maximizing) was won by the circle. But if the fixed perimeter is measured by the line integral of $|dx| + |dy|$, a square would win. Or if the boundary integral of $\max(|dx|, |dy|)$ is given, a diamond has maximum area. For any norm in R^2, we show that when the integral of $||(dx, dy)||$ around the boundary is prescribed, the area inside is maximized by a ball in the dual norm. This has application to computing minimum cuts and maximum flows in a plane domain.

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MS23

Introduction/Overview/Historical Perspective

Over his fifty years of professional life, Ben Noble (1922-2006) made many outstanding contributions (both research and teaching) to several areas of applied mathematics. After a distinguished career at the Admiralty Research Laboratory, United Kingdom, during the World War II, he embarked on an active academic career. Since his migration to US in 1962, Professor Noble devoted his professional life to research on a variety of applied mathematical topics that continue to be highly relevant to Defense Science Technology. In this symposium, former students, collaborators, associates, and friends of Noble will review some of these topics; evaluate the logical evolution of these areas and their impact on contemporary applied mathematics.

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MS23

Numerical Methods for Integral Equations

Amongst his many contributions to numerical analysis, Ben Noble had a great impact on the development of numerical methods for the solution of integral equations. Through his own work and the work of his students he created an interest in this topic that brought it from relative obscurity to an active area of research with many applications. This talk will trace the development of integral equation methods from the early 1960s to the present time.

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MS23

Ben Noble and the Changes in Teaching Linear Algebra

The teaching of linear algebra has changed more significantly, and in more universities, than any other subject in undergraduate mathematics. From the beginning, Ben Noble played a very important and constructive part. His textbook pointed the way, and later editions with Jim Daniel were major steps forward to a course that meets the needs of students. We will talk informally about this change from "abstract" to "concrete". Instead of teaching proofs we are closer to communicating ideas. The mathematical content does not suffer, most students learn more.

Linear algebra is a beautiful subject and this is a happy chance to offer students a course that they can use and even enjoy.

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MS24

A Fully Implicit R-refinement Algorithm

R-refinement techniques rely on suitable grid equations to guide mesh motion. Such grid equations are generally stiff, making its numerical inversion a challenge. Furthermore, R-refinement methods typically split the mesh motion from the physics, resulting in grid lagging. We propose an R-refinement algorithm based on the Laplace-Beltrami formulation that efficiently inverts the coupled grid-physics system. We will demonstrate that the algorithm is both efficient (cost effective vs. uniform grid approaches) and scalable under grid refinement.

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MS24

Planar, Surface, and Volume Mesh Generation using the Laplace-Beltrami Target Metric (LBTM) Method

The Laplace-Beltrami equations have recently been considered for the generation of quasi-conformal meshes in two- and three-dimensional applications. These equations allow the specification of mesh characteristics by using an approximate metric tensor. Indeed, it is often possible to prescribe final mesh criteria by forming, on an element by element basis, an ideal target element representation that is based upon local modification of the existing mesh state. The use of a prescriptive target metric as a solution-dependent diffusion tensor in the Laplace-Beltrami procedure results in the LBTM method; an elliptic mesh generation method that is robust with respect to domains containing complex convex or concave boundaries. This presentation discusses the mechanics of the LBTM method and its application to selected example problems.

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MS24

R-refinement Within the Target-Matrix Paradigm

A matrix-based approach to mesh quality optimization is presented in which 'target' matrices describe application-specific mesh quality. The paradigm provides a general framework to guide mesh optimization for a variety of mesh improvement and adaptive problems, including r-refinement. For r-refinement, target matrices are computed from local error estimates or indicators, most prominently using approximations to the solution Hessian. The paradigm shifts focus away from mesh quality metrics toward the design of automatic target-matrix calculators.

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MS24

The New Error Minimization Based Moving Mesh Method: Theoretical andNumerical Analysis

We describe and analyze a moving mesh method for fluid flow. A typical moving mesh method includes an optimal mesh criterion, an error indicator or estimator, and a strategy for mesh improvement. We apply the standard a posteriori error estimate and minimizes the L2-norm of error over a set of smooth meshes which is our mesh improvement strategy. The results of analysis will be used to explains common features of a few other moving mesh methods. The proposed method improves accuracy of the numerical solution of the system of 1D gasdynamics equations. Extension of the method in 2D will be also discussed and illustrated with preliminary results.

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MS25

Modeling Human Papillomavirus (HPV) Transmission, Cervical Cancer Development, and Impact of HPV Vaccines in an Age-structured U.S. Population

Abstract not available at time of publication.

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MS25

Optimal Peptide-based Vaccination for HTLV-I Infection

Human T-lymphocyte virus type I (HTLV-I) is the causative agent of HTLV-I associated myelopathy (HAM) and other illnesses. Clinical evidence suggests that the mitotic expansion of infected clones plays a relevant role in the infection dynamics. The use of peptide-based vaccines that target those rapid proliferating clones has been clinically suggested. We consider a mathematical model for peptide-vaccination regime for HTLV-I and analyze an optimal control mechanism for such vaccination procedure.

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MS25
Host Extinction Dynamics in Epidemiology Models

This talk begins by presenting a simple SI model for formulated through the basic birth and death processes. Complete mathematical investigation of this simple model shows that the host extinction dynamics can happen and the outcomes may depend on the initial conditions. We also present some extensions of this model to structured SI models, including delay differential equation SI models. We show that host extinction dynamics is ubiquitous to many well formulated epidemiology models.

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MS25
Optimal Control for Management of an Invasive Plant Species

We consider the management of the spread of invasive plant populations consisting of a large main focus and several smaller outlier populations. We formulate a discrete time model to determine the optimal control strategy, including a constraint on the total amount of control applied.

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MS26
Phases and Aquatic Locomotion: Wake-body Interactions

Irrotational inviscid flow models and Stokes flow models fail to account for the generation of dynamic vortex wakes by moving bodies, a phenomenon central to locomotion in water on a macroscopic scale. This talk will describe some reduced models for capturing the dynamic interaction of fish with the wake vorticity.

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MS26
Phases and Aquatic Locomotion: Driftless Swimming

Symmetries exhibited by idealized models for the locomotion of deformable bodies in fluids provide for the definition of principal connections which encapsulate relationships between body deformations and resulting translations and rotations in space. It follows that issues of controllability and motion-planning for such systems can be addressed in terms of geometric phases. This talk will describe the geometric treatment of swimming in the driftless extremes of irrotational inviscid flow and Stokes flow.

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MS26
Lie Group Variational Integrators and Discrete Under-actuated Optimal Control Problems

We introduce Lie group variational integrators, which are based on a discretization of Hamilton's principle that automatically remain on the Lie group without the use of local charts, reprojection, or constraints. In particular, these yield highly efficient geometric integration schemes for rigid body dynamics. We will address the application of these numerical methods to the control of the 3D pendulum system, and the role of geometric phases in the study of under-actuated control problems.

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MS26
Applications of Geometric Phases in Classical Mechanics: Molecular Dynamics

In N-body systems from macromolecules to triatomic molecules, internal motions can produce an overall rotation often neglected yet explainable by a geometric phase. The overall rotation has been observed in molecular dynamics simulations of protein molecules at zero total angular momentum. This overall rotation is also described for triatomic molecular systems with either normal modes or large-amplitude motions. These situations provide examples of geometric phases occurring more generally in classical systems.

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MS27
Hyperbolic Systems with Dissipation

Global weak solutions of a strictly hyperbolic system with dissipative source are constructed via the vanishing viscosity method. Moreover, we establish sharp estimates on the uniformly Lipschitz semigroup generated by the vanishing viscosity limit in the general case which includes also nonconservative systems and prove uniqueness of solutions by means of local integral estimates, which shows that every viscosity solution can be constructed as a limit of vanishing viscosity approximations.

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MS27

Patterns on Growing Square Domains via Mode Interactions

We consider reaction-diffusion systems on growing square domains with Neumann boundary conditions (NBC). As suggested by numerical simulations, we study the simpler problem of mode interactions in steady-state bifurcation problems with both translational symmetry and square symmetry, combined with the symmetry constraint imposed by NBC. We show that the transition between different types of squares can be generically continuous. Also, we show that transitions between squares and stripes can occur generically via a jump, via steady-states or via steady-states and time-periodic states. We point out some differences between stable patterns in the NBC problem and in the periodic boundary conditions problem. This is joint work with Martin Golubitsky.

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MS27

Irregular to Regular Sampling, Deconvolution, Denoising and Zoom

We propose an algorithm to solve a problem in image restoration which considers several different aspects of it, namely: irregular sampling, denoising, deconvolution, and zooming. Our algorithm is based on an extension of a previous image denoising algorithm proposed by A. Chambolle using total variation, combined with irregular to regular sampling algorithms proposed by H.G. Feichtinger, K. Grchenig, M. Rauth and T. Strohmer. The proposed variational problem incorporates local constraints in order to preserve textures and flat zones.

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MS27

An Asymptotic Framework for Finite Hydraulic Fractures Driven by Multiple Physical Processes

A novel asymptotic framework is presented to describe hydraulic fracture propagation. The problem consists of a system of nonlinear integro-differential equations, with local and nonlocal effects. This causes transitions on a small scale near the fracture tip, which control the behavior across the whole profile. These transitions depend upon dominant physical process(es), and are identified by simultaneously scaling the associated parameters with the distance from the tip. An analytic solution incorporating several processes is obtained.

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MS28

An Asynchronous Parallel Algorithm for Handling General Constraints in the Context of Generating Set Search Methods for Derivative-free Optimization

We will discuss an asynchronous parallel implementation of a derivative-free augmented Lagrangian algorithm for handling general nonlinear constraints. Our primary focus will be on solving problems whose objective and/or constraint functions are computationally expensive. The method solves a series of linearly constrained subproblems, seeking to approximately minimize the augmented Lagrangian which involves the nonlinear constraints. Each subproblem is solved using a generating set search algorithm capable of handling degenerate linear constraints. We use APPSPACK to solve the linearly-constrained subproblems, enabling the objective and nonlinear constraint functions to be computed asynchronously in parallel. A description and theoretical analysis of the algorithm will be given followed by extensive numerical results.

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MS28

Implicit Filtering and Applications

Implicit filtering samples the objective function at a stencil of points centered at the current best point. The optimization is governed by a finite difference quasi-Newton step and the results of a direct search on the stencil. In this talk we describe a new implementation of implicit filtering in MATLAB, some new convergence results, and the application of the new code to a problem in hydrology.

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MS28

An Augmented Lagrangian Pattern Search Algorithm for Linear and Nonlinear Constrained Optimization

This talk demonstrates a pattern search algorithm for linear and nonlinear constrained optimization. Our approach is motivated by the bound constrained augmented Lagrangian algorithm for pattern search by Michael Lewis and Virginia Torczon. Our implementation handles linear and bound constraints separately from the nonlinear constraints. A sub-problem is formulated by combining the objective, the nonlinear equality, and the nonlinear inequality constraint functions using Lagrangian and penalty parameters. A sequence of such optimization problems are approximately minimized using the pattern search such that the linear and bounds constraints are satisfied. The subproblem formulation and the update of Lagrangian and penalty parameters is an adaptation of work by Conn, Gould, and Toint on augmented Lagrangian methods. We give numerical results for this method on several test problems.

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MS28

Constrained Optimization by Generating Set Search

We discuss an augmented Lagrangian approach to applying generating set search to nonlinear programming. The approach is based on the approximate minimization, with a suitable derivative-free stopping criterion, of a sequence of augmented Lagrangian relaxations of the original problem, with bound and general linear constraints kept explicit. We highlight the analytical results underlying the approach and provide numerical illustrations. We also discuss strategies for active set identification and techniques for accelerating the overall optimization process.

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MS29

Flow Models of Ferroelectric Liquid Crystals

This presentation deals with modeling of nonlocal electrostatic effects in liquid crystals. While many of the liquid crystals found in applications are dielectric, the synthesis of new materials, such as the bent-core molecule type, motivate studies of ferroelectric phases. The spontaneous polarization of the liquid crystal creates an electrostatic energy that may be felt in the whole space. Molecular and shape rearrangement take place in order to prevent energetically costly configurations. We will discuss bulk rearrangements in terms of undulation and periodicity. Likewise, we argue that the development of telephone cord shapes observed in bent-core molecule liquid crystal filaments is also the result of an optimization mechanism. We will discuss the formation of helical filaments from the point of view of nonlinear elasticity. We will end the presentation addressing related flow phenomena.

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MS29

Numerical Modeling of Electric-field-induced Transitions in Cholestric-liquid-crystal Films

We consider thin films of a cholesteric liquid-crystal material subject to an applied electric field. In such materials, the liquid-crystal ”director” (local average orientation of the long axis of the molecules) has an intrinsic tendency to rotate in space; while the substrates that confine the film tend to coerce a uniform orientation. The electric field encourages certain preferred orientations of the director as well, and these competing influences give rise to several different stable equilibrium states of the director field, including spatially uniform, translation invariant (functions only of position across the cell gap), and periodic (with 1-D or 2-D periodicity in the plane of the film). These structures depend on two principal control parameters: the ratio of the cell gap to the intrinsic ”pitch” (spatial period of rotation) of the cholesteric and the magnitude of the applied voltage. We report on numerical work (in progress) on the bifurcation and phase behavior of this system. The study was motivated by potential applications involving switchable gratings and eyewear with tunable transparency. We compare our results with recent experiments conducted in the Liquid Crystal Institute at Kent State University

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MS29

Hydrodynamics inside the Lung: Materials, Forces and Flows

Abstract not available at time of publication.

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MS29

Kinetic Model Simulations of 2-d Structure Formation in Sheared-rigid Rod Suspensions

We present a numerical algorithm for nano-rod suspension flows, and provide benchmark simulations of a plane Couette cell experiment. The system consists of a Smoluchowski equation for the orientational distribution function of the nano-rods together with the Navier-Stokes equation for the solvent with an orientation-dependent stress. The rigid rods interact through nonlocal excluded-volume and distortional elasticity potentials and hydrodynamic interactions. The algorithm resolves full orientational configuration space, two dimensional physical space, and time, and employs a velocity-pressure formulation of the Navier-Stokes equation. This method extends our previous solver from 1D to 2D in physical space.

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MS30

Conformal Cortical Cartography Using the Discrete Approach of Circle Packings

The functional processing of the human brain occurs on the highly fold surface, called the gray matter. Neuroscientists are interested in developing 2D, surface-based analysis methods for analyzing the location of functional processing and studying disease and aging. Our group was the first group to propose using conformal-based methods for unfolding and flattening the cortical surface. We compute our quasi-conformal maps using circle packings and since then, a number of other conformal-based approaches have been suggested. I will discuss the method of circle packings, how we are applying it to brain imaging and open questions which need to be investigated.

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MS30

Automatic Detection of Anatomical Features Using Brain Conformal Parametrization

Important anatomical features on the cortical surface are usually represented by landmark curves, called sulci/gyri curves. Manual labelling of these landmark curves is time-consuming, especially when there is a large set of data. In this paper, we propose a method to trace the landmark curves on the cortical surfaces automatically based on the principal directions. Suppose we are given the global conformal parametrization of the cortical surface, our method traces the landmark curves iteratively on the spherical/rectangular parameter domain along the principal direction, which is based on a variational approach. This involves solving a PDE on the cortical surface. Consequently, the landmark curves can be mapped onto the cortical surface. To speed up the iterative scheme, we propose a method to get a good initialization by extracting the high curvature region on the cortical surface using Chan-Vese segmentation method, which involves solving another PDE on the surface. Using the global conformal parametrization technique, we propose a method to solve PDEs on surfaces with arbitrary topologies. The main idea of this method is to map the surface conformally to a 2D rectangle and then transform the PDE on the 3D surface into a modified PDE on the 2D parameter domain. Consequently, we can solve the PDE on the parameter domain by using some well-known numerical schemes on $\mathbb{R}^2$. To do this, we have to define a new set of differential operators on the manifold such that they are coordinates invariant. Since the Jacobian of the conformal mapping is simply a multiplication of the conformal factor, the modified PDE on the parameter domain will be very simple and easy to solve. Experimental results show that the landmark curves detected by our algorithm closely resemble to those manually labelled curves. As an application, we used these automatically labelled landmark curves to build average cortical surfaces with an optimized brain conformal mapping method. Experimental results show our method can help automatically matching brain cortical surfaces.

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MS30

Computational Methods for Quantitative Analysis of the brain

This talk will summarize our work on analysis of MR brain images. Our main research goal aims at developing automated image analysis methods for precisely quantifying subtle and complex structural/ functional changes in the brains, to be used for early detection of brain diseases, such as Alzheimer's Disease (AD). Accordingly, we developed a 3D brain registration method, called HAMMER, which has been successfully applied to many large clinical research studies and clinical trials, involving approximately 3,000 MR brain images. Moreover, we developed a nonlinear brain classification method to jointly use all structural changes for classification of schizophrenia patients from normal controls. Details of HAMMER registration algorithm and nonlinear brain classification method will be discussed in this talk.

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MS30

Brain Mapping Techniques for Computer Aided

Diagnosis and Follow Up

In this talk, we will present an integrated neuroimage processing pipeline being developed in our Center for computer-aided clinical diagnosis and follow-up of neurological disorders patients. The pipeline is strongly grounded on a number of mathematical brain mapping techniques, including high-dimensional hybrid volumetric and surface warping; cortical surface reconstruction, nonlinear image registration, statistical modeling, conformal mapping and visualization, whole brain parcellation, and quantitation of diffusion tensor imaging and gray matter diffusivity. These mathematical techniques have been applied to aid the diagnosis and monitoring of patients with Creutzfeldt-Jakob disease, Alzheimers disease, schizophrenia, primary brain tumor, and adolescent idiopathic scoliosis. We will report our experimental results from some of these clinical studies.

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MS31

Extension of the Principal Interval Decomposition for Model Reduction in Fluids

The Principal Interval Decomposition is an extension of POD that can identify solution modes that are dominant over short time intervals, but would be missed by standard POD. We investigate the role of the PID in generating bases for reduced order models of nonlinear problems using an example from fluid flow.

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MS31

Model Reduction and the Solution of Sylvester Equations

In this paper, we derive a reliable way to compute the orthogonal bases of the generalized Krylov subspaces required for model reduction via tangential interpolation. The residual error of the large linear systems of equations that are solved in order to produce the bases are controlled so as to yield a small backward error in the associated Sylvester equations and in the model reduction problem. The efficiency and effectiveness of the algorithm is also discussed.

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MS31

Approximate Solution of Lyapunov Equations in Low Rank Factored Form

An algorithm is presented to approximately solve large scale Lyapunov equations in low rank factored form. The algorithm is based upon a synthesis of an approximate power method (APM) and an alternating direction implicit (ADI) method. The new algorithm uses an APM correction step to obtain a basis update and then constructs an appropriate re-weighting of this correction to provide a factored update that enjoys ADI-like theoretical convergence properties. The method converges rapidly in practice.

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MS31

Model Reduction for Large-Scale Systems with High-Dimensional Parametric Input Space

A key challenge that must be addressed to obtain reduced-order models for large-scale optimal design, optimal control, and inverse problem applications is the need to capture variation over a parametric input space of high dimension. We pose the task of determining appropriate sample points for a reduced basis method as an optimization problem, which is implemented using an efficient adaptive algorithm that scales well to systems with a large number of parameters.

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MS32

Incoherent Solitons in Instantaneous Nonlinear Media

Spatially incoherent solitons self trap entities whose structure varies randomly in time form when diffraction is robustly balanced by self-focusing. This balance results in the stationary propagation of the beams envelope. Until recently, it was believed that a prerequisite for the formation of incoherent solitons is that the nonlinearity is noninstantaneous having a response time much longer than the characteristic beam fluctuation time. We present our study on incoherent solitons in instantaneous nonlinear media.

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MS32

Mode Competition in Bragg Grating Defects

We consider light confined by a defect in a Bragg grating optical fiber that supports multiple bound states. This system has no energy-minimization principle, but selects a sort of ground state when more than one mode is initialized. The interaction takes place via coupling to the continuous spectrum. Eigenvalues are computed numerically using Evans functions. Instabilities arise due to edge bifurcations and to collisions between neutral eigenvalues colliding with the continuous spectrum.

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MS32

A Hierarchy of Homoclinic Bifurcations at the Onset of Pulse Self-Replication

We establish a series of properties of symmetric, N-pulse, homoclinic solutions of the *reduced* Gray-Scott system

$$u'' = uv^2, \qquad v'' = v - uv^2,$$

which play a pivotal role in questions concerning the existence and self-replication of pulse solutions of the full Gray-Scott model. Specifically, we establish the existence, and study properties, of solution branches in the (α, β)-plane that represent multi-pulse homoclinic orbits, where α and β are the central values of $u(x)$ and $v(x)$, respectively. We prove bounds for these solution branches, study their behavior for large α , and establish a series of geometric properties of these branches which are valid throughout the (α, β)-plane. We also establish qualitative properties of multi-pulse solutions and study how they bifurcate, *i.e.*, how they change along the solution branches.

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MS32

Numerical Study of One-dimensional Bose-Einstein Condensates in a Random Potential

We present a detailed numerical study of the effect of a disorder potential superimposed on a confining trap on a one-dimensional Bose-Einstein condensate in the framework of a mean-field description, i.e., Gross-Pitaevskii equation. We find that the ensemble average size of the stationary profile decreases with an increasing strength of the disorder potential for repulsive as well as attractive interactions among atoms. For repulsive interactions, when the trap is switched off, with the increasing strength of disorder, an inhibition of the expansion of the condensate occurs both in the interaction dominated Thomas-Fermi regime and the confinement dominated Gaussian regime. However the details of the time dependent profile differ considerably in these two situations.

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MS33

Efficient Cluster Computing for Time-Dependent Reaction-Diffusion Equations on High Resolution Meshes

The flow of calcium ions in one human heart cell can be modeled by a system of time-dependent reaction-diffusion equations. The flow is driven by sources at a large number of discrete points in the three-dimensional domain that necessitate the use of meshes with millions of nodes. The use of parallel computing clusters allows for the solution of this problem with excellent scalability on a commodity cluster with a high-performance computational interconnect.

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MS33

Tracking the High End of Mesh-based PDE Simulations through the Gordon Bell Prize

The Gordon Bell Prize, awarded annually since 1988 for high sustained floating point rates on real applications, has often attracted submissions based on finely resolved meshes that arise from multiscale PDEs or fundamentally lattice-based phenomena. Since 1999, the Special Prize has been awarded for simulations that fall short of highest sustained flop/s, but define new performance envelopes for mesh-based applications with irregular data access patterns. We review the applications and hardware intertwined in this history, extrapolate trends, and look in detail at recent noteworthy submissions.

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MS33

Parallel Hybrid Solvers for Large Scale Finite Element Problems

We consider the development of hybrid preconditioners that can accelerate the convergence of parallel Conjugate Gradients for systems from finite element applications. Our hybrids exploit tree-structured parallelism to combine the strengths of incomplete Cholesky factorization and sparse approximate inversion schemes. We will discuss our hybrid scheme and provide empirical results on the quality of preconditioning and execution times for preconditioner construction and application on large-scale multiprocessors.

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MS33

Parallel Solution of a Finite Element Problem with 10 Billion Unknowns

Large-scale, parallel, finite element simulations require scalable algorithms, such as the multigrid method and a careful design and analysis of their implementation. This includes identifying and removing bottlenecks that limit the serial performance of component algorithms such as smoothing and residual error calculation. The Hierarchical Hybrid Grids (HHG) framework has been developed as an efficient, memory conserving data structure for multilevel algorithms that exploits the regularity of very fine meshes after repeated refinement. The HHG algorithms and data structures show excellent serial performance and equally good parallel scalability. The HHG framework has been implemented on a 1024 processor SGI Altix to solve large finite element problems with more than ten billion unknowns.

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MS34

How Stability Leads to Variability: An Example from Gene Expression

Abstract not available at time of publication.

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MS34

Interaction of Motor Proteins with Obstacles

Motor proteins frequently interact with obstacles in the crowded cellular environments. We consider systems in which two degrees of freedom, the motor protein and the obstacle, affect each other's motion. Examples include helicase unwinding of DNA, a polymerizing filament which grows near a wall, and two motor proteins colliding on a microtubule. This talk describes a simplified model of the motor protein-obstacle interaction, where an interaction potential describes how the protein and obstacle affect each other's motion. Results are presented both for the general model and for the specific problem of helicases, the motor proteins which unwind double-stranded DNA in cells. We show that the form of the interaction between helicase and junction strongly affects the overall DNA unwinding rate.

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MS34

A Multi-Scale Approach to Brownian Motors

The problem of Brownian motion in a periodic potential, under the influence of external forcing, which is either random or periodic in time, is studied in this paper. Multiscale techniques are used to derive general formulae for the steady state particle current and the effective diffusion tensor. These formulae are then applied to calculate the effective diffusion coefficient for a Brownian particle in a periodic potential driven simultaneously by additive Gaussian white and colored noise. Our theoretical findings are supported by numerical simulations.

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MS34

A Unified Framework for Modeling the Dynamics of Signaling Pathways

The emergence of high throughput technologies for molecular biology is making the study of biochemical signaling networks a possibility. However, as more signaling networks and elements are being identified, their complexities and the intricate interactions among signaling molecules, or cross-talk, are quickly becoming intractable. Understanding how cells do signal processing therefore requires models that define layers of abstractions in order to view signaling algorithms at different resolutions. While a number of deterministic and stochastic models have been formulated over the years to describe different aspects of the dynamics of signaling networks, most of these models use different formalisms and concepts making their integration into a unified framework very difficult. Here, we introduce a new framework for modeling cellular signal processing based on interacting Markov chains. This framework provides a unified way to simultaneously capture the stochasticity of signaling networks in individual cells while computing a deterministic solution which provides average behavior therefore allowing modeling at multiple resolutions within the same framework. The use of this framework is demonstrated on two classical signaling networks: the Mitogen Activated Protein Kinase (MAPK) cascade and the signaling pathway underlying bacterial chemotaxis.

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MS35

Rate of Convergence of Numerical Solutions for Stochastic Partial Differential Equations

In this talk we will present some of the recent developments on numerical solutions for stochastic partial differential equations (SPDEs). We will focus on the error estimates of 1. The stochastic spectral finite element method for SPDEs with random coefficients; 2. Galerkin approximation for SPDEs with white noise forcing term; We will also discuss the challenges of numerical implementations of the approximate solutions.

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MS35

Scaling Behavior of Stochastic, Multiphase Flow in Porous Media

It has become increasingly apparent that subsurface formations are heterogeneous at all length scales, and that fine scale heterogeneities, particularly in the permeability field, can have a significant impact on large scale flow. Due to the difficulty in complete and certain characterization of these heterogeneities, stochastic representations of subsurface geologic properties have become commonplace. As a result, the flow equations have stochastic coefficients, and must also have stochastic solutions. Thus predictions of flow outcomes are inherently stochastic. We examine multiphase flow in stochastically described heterogeneous porous media. The study centers on the interplay between nonlinearity and heterogeneity in determining fluid mixing dynamics. Monte Carlo simulations are used for a quantitative analysis of this mixing. Different flow regimes, identified by the large time scaling behavior of the mixing deynamics, are characterized. This characterization provides significant guidance for uncovering effective methods (and their limits) for the scaling-up of multiphase flow systems to scales suitable for computationally inexpensive yet accurate fluid flow simulations.

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MS35

Stochastic Multi-Scale Methods for Turbulent Flow Simulations

The use of stochastic methods for turbulent flow simulations has significant advantages compared to the application of deterministic methods: the important effects of sources (chemical reactions) can be treated exactly, and the mechanism of turbulent fluctuation dynamics is explained (which is also helpful to develop consistent closures for correlations of turbulent variables that appear as unknowns in deterministic equations). However, stochastic methods developed previously are, basically, only applicable to certain scales: the molecular scale, small-scale turbulent motions (filter density function methods) and large-scale turbulent motions (probability density function methods). First, the paper illustrates these methods and their characteristic advantages and disadvantages by means of several examples. This discussion results in the conclusion that methods should be developed that have a broader range of applicability, this means we need methods which are applicable to a variety of scales. The second part of this paper shows how it is possible to develop such stochastic multi-scale methods. The capabilities of such multi-scale methods and some remaining challenges are described finally.

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MS35

Approximation of SPDE's of Wick Type by Finite Element and Finite Volume Methods

Stochastic partial differential equations (SPDEs) play fundamental and important roles in many problems. Their mathematical treatment is more involved compared to that of deterministic partial dierential equations. Their numerical simulations become an important strategy in practical applications. We propose the development of fnite element and finite volume approximations of SPDEs, particularly those SPDEs modelling fluid flows such as the stochastic pressure equations or the stochastic Navier-Stokes equations that involve additive and multiplicative white noises via the Wick product. We give existence and uniqueness results for the continuous problem and its approximation by finite element method. Optimal error estimates are derived and algorithmic aspects of the method are discussed. Our method will reduce the problem of solving SPDEs by solving a set of deterministic ones. Moreover, one can reconstruct particular realizations of the solution directly from Wiener chaos expansions once the coecients are available. Finally, we present numerical results of some test problems.

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MS36

Grid-Free Lagrangian Laser Plasma Simulations

Modeling and simulation of intense laser plasma interactions has gained significant recognition due to advances in inertial confinement fusion, nondestructive materials testing, wake field accelerators, etc. In many of these systems, the plasma is simulated using a Lagrangian descriptions, i.e., the plasma is modeled as a collection of macro particles in phase space evolving under the action of an external force. In this work we consider the development of a grid-free Lagrangian plasma simulation for the self-consistent simulation of laser plasma interactions. The method is O(N log N) and couples a treecode field solver with a boundary integral method. The method has advantages over traditional mesh based methods, as has been discussed in our earlier work. As a first step to developing a grid-free electromagnetic laser plasma model, we model the laser plasma interaction electrostatically as a ponderomotive force. We then compare the grid-free solution to one computed using a traditional mesh based method.

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MS36

Virtual Prototyping of High Power Microwave Devices using a Massively Parallel Electromagnetic

Particle-in-Cell Code

We are performing virtual prototyping of RF systems, from pulse power through to antennas, with the ICEPIC (Improved Concurrent Electromagnetic Particle-in-Cell) HPC software that we have developed over the past several years with funding from AFOSR. This code simulates from first principles (Maxwells equations and Lorenzs force law) the electrodynamics and charged particle dynamics of HPM systems. The simulations that are used to design these tubes can contain over a billion cells, more commonly around a 100 million. This talk will focus on the electron emission models used at the cathode and weighting of the particles motion to the grid as currents. The impact of improving the algorithms for emission and current weighting is quantified by the improvement of accuracy and decrease in time to solution for these large design simulations as well as simple 2d test problems.

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MS36

Implicit Moment Particle In Cell (PIC) Simulation of Multiple-Scale Plasma Simulation

Kinetic PIC methods are limited by their need to resolve the smallest scales in space and time for stability. We describe the latest implementation of the implicit moment method for kinetic PIC simulation. The primary features are: 1) elimination of the explicit stability constraint, the time step and the grid spacing are limited by an accuracy condition; 2) several orders of magnitude can be gained in CPU time for a given accuracy; 3) Large scale macroscopic kinetic simulations becomes feasible.

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MS36

Particle Simulations with 2nd-order Accurate Field Algorithms in the VORPAL Plasma Simulation Software

We give an overview of the VORPAL plasma simualtion software and recent improvements which allow for 2nd-order accurate FDTD field solutions in complex structures with curved surfaces. Implementation, benchmarking, and analysis of Dey-Mittra and Zagorodnov cut-cell algorithms is presented. The VORPAL software contains several particle simulation methodologies, including particle-in-cell (PIC), DSMC, and delta-f methods. Issues involving particle creation, kill, and interactions in the cut-cells will be discussed, and progress in these areas will be presented. Use of 2nd-order accurate algorithms with particles is illustrated for accelerator cavity and other complex geometries, using large-scale parallel computing resources. Funding for this work provided by AFOSR Contract FA9550-04-C-0041, and DOE Contracts DE-FG02-05ER84172 and DE-FG02-03ER83841.

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MS37

Modelling the Hiv/AIDS Epidemic in Sub-Sahara Africa: The Effects of Interventions

In Sub-Sahara Africa the population can be divided into high-risk and low-risk subgroups. We investigate the effectiveness of intervention focused on reducing the burden of HIV/AIDS among high-risk individuals. Within decades drug resistance will be widespread and the epidemic will continue unabated. Accordingly, we address the problem: at what rate and at what stage should HIV/AIDS patients be treated to ensure that the current drugs remain useful until the next generation of drugs is developed?

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MS37
Vaccine Induced Pathogen Type Replacement

Many pathogens are represented by multiple antigenically distinct types. Vaccination provides vaccinated individuals with immunity specific to the particular type that created it. What is observed on population level when a vaccination campaign is initiated is that those pathogen types that circulated in the population before the vaccination diminish in prevalence while others (typically not included in the vaccine) increase in prevalence. This phenomenon has been termed the replacement effect. The mechanism of the replacement effect is thought to be the differential effectiveness of the vaccine. In a recent article we reported that we observed population level strain replacement in an epidemic model with super-infection and "perfect" vaccination, that is vaccination that protects 100 percent all vaccinated individuals against both strains involved in the model. Would strain replacement have occurred if the trade-off mechanism in the model was not super-infection but coinfection and the vaccine is perfect? If differential effectiveness of the vaccine is not necessary for the replacement effect to occur, what is the causal mechanism of strain replacement? How does that mechanism explain the occurrence of the effect in the presence and in the absence of differential effectiveness of the vaccine? I will address these questions in this talk.

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MS37
Stability for a Class of Epidemic Models with Mass Action Incidence

An ODE mass action model of tuberculosis with an arbitrary number of latent stages is considered, allowing a very general distribution of latency times to be approximated. The global dynamics of the system are completely determined, yielding the traditional threshold behaviour. The results are extended to the limiting case where the number of latent classes goes to infinity, giving results for PDE and integral equation systems.

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MS37
Construction of Dynamical Consistent Finite Difference Schemes for ODE's Modeling Biological Systems

Mathematics plays an essential role in the understanding of various phenomena in the biological/biomedical sciences by its use both to formulate models of the underlying dynamics and the subsequent application of techniques to study the evolution of the system variables. However, the complexity of the derived differential equations generally do not allow the calculation of explicit solutions. A consequence of this situation is the need to have integration methods that permit valid numerical solutions to be calculated. A popular technique, widely used in the natural and engineering sciences, is based on the use of finite differences to approximate the derivations and other functions occurring in the differential equations. Using the concept of dynamical consistency, we demonstrate that valid discrete models of differential equations can be constructed. In addition to introducing the concepts and methods of NSFD schemes, their utility is demonstrated by applying these techniques to several important systems of coupled, nonlinear ODE's modeling biological/biomedical systems. This work has been supported in part by a research grant from DOE.

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MS38
High Frequency Sparse Array Synthesis for Target Identification Signatures

It is known that high frequency in the terahertz (THz) range have some unique advantages. They have high reflective properties for biological objects and have a good penetration property through dielectric materials. These radiations are non-ionizing and can be used for civilian applications. High frequency aperture consisting of THz transmission modules can be fairly small allowing the equipment to be portable. Phased array components mainly consist of sources detectors up-converters down-converters mixers and circulators. These components, for THz applications, are under active development. However each component of these high frequency modules for transmission and reception can be fairly large. In this paper thinned phased arrays have been investigated. A deterministic approach involving space tapering using Taylor synthesis for continuous aperture has been used. Discretization has been carried out and performance of these arrays has been evaluated for various side-lobe controls. Circular as well as elliptical arrays have been considered. Using the results of thinned circular discrete array elements, elliptical arrays have been designed using invariant principal of the synthesis and their performance evaluated. Use of these arrays for generation of signatures for target identification has been indicated.

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MS38
Reflections on Ben Nobles Contributions to Generalized Inverses,

Ben Noble and I discussed on many occasions generalized inverses of matrices and related aspects of integral equations of the first kind. He told me once that he is only a dabbler in this area who wants to learn more. I have learned from Ben more than he has learned from me. Ben had strong views on usefulness and strong limitations of various formulas for matrix generalized inverses and computational methods. In this talk, I will reflect on some of Ben Nobles contributions to generalized inverses and reminisce about some discussions and encounters.

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MS38

Analysis of Inexact Inverse Iteration for Large Sparse Eigenvalue Problems Using Newton's Method with Application to Preconditioned Iterative Solvers

The use of Newton's method to discuss inverse iteration was first considered by Unger in 1950 (ZAMM,vol 30,pp281-282) and was rediscovered by Wilkinson in the early 1970's, though the most well-known article didn't appear until 1979 (Peters and Wilkinson, SIAM Rev). Ben Noble told me about Wilkinson's idea in 1972 and my PhD thesis in 1974 contained an appendix developing this idea. Since then similar ideas have been used to great effect to derive numerical methods for nonlinear eigenvalue problems and bifurcation problems. Very recently this way of looking at inverse iteration as a Newton method has proved helpful in analysing the convergence of inexact inverse iteration for large sparse matrix eigenvalue problems. In such problems it is often impractical to solve the shifted linear systems directly and iterative methods are employed to solve systems to a specified tolerance. In this talk a convergence analysis for inexact inverse iteration using variable shifts and fixed or varying solve tolerances will be given. A useful byproduct of the analysis is that it suggests a new approach to the problem of preconditioning the shifted systems that arise in inverse iteration. Numerical examples will be given.

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MS38

Mixed Boundary Value Problems and Singular Integral Equations

Some classical problems from dual integral equations and singular integral equations with Cauchy-Principal -Value integrals are revisited in the context of uncertain data , instability and lack of uniform convergence.

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MS38

On Generic Convergence of Numeical Methods for Hybrid Dynamical Systems

We consider the initial value problem for a large class of impulsive and hysteretic hybrid systems. We define a geometrically intuitive metric on a suitable space of cadlag functions, then construct numerical approximations that converge generically (but not necessarily generally) in this metric. We conjecture that the metric used generates the Skorohod J-1 topology.

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MS39

Model Selection as an Inverse Problem

In the literature of infectous diseases, it is common to find multiple proposed models for the same pathogenic phenomena. In many of these cases, the models are systems of differential equations, which the authors then fit to experimental data to infer conclusions about the biological system. We propose a model selection methodology which includes models for deterministic individual dynamics and random population effects. These are combined in a model selection criterion which balances goodness-of-fit with a measure of statistical complexity. The inverse problem concerning the distinguishability of a class of models will be discussed. Analytical and computational results will be presented as well as an application to modeling *in vivo* HIV infection dynamics under therapy.

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MS39

Using Sensitivity Analysis and Fisher Information in the Design of Viral Dynamics Studies

Abstract not available at time of publication.

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MS39

Back to the Basics to Improve our Ability to Model Infectious Diseases

Infectious disease modeling has become one of the hottest topics in mathematical biology. However, to apply mathematical models to infectious disease dynamics can be quite tricky and complicated. Since there are no natural physical laws that we can utilize, like those in cancer and developmental biology modeling, one must begin to look at traditional mathematical concepts to address model correctness. Fortunately, there are some wonderful tools avialable, such as model sensitivity, model selection, and model identifiability, that we can use. In this talk I will discuss the reasons for the use of these tools and how these tools help improve our modeling capabilities. Our group has been working on developing algorithms for identifiabiliy and selection that hopefully will make it easier for modelers to employ these techniques in their work. I will focus on models for HIV and HBV dynamics and show the ways that we can improve upon our modeling of these diseases. For instance, numerous models have been used to predict parameters from patient data in HIV but applying a simple technique from algebra, called model identifiability, we have been able to show that the models we have been using are not necessarily identifiable. Hence, we are working to put modeling of ID on solid ground using these techniques. We will also discuss techniques from statistical methods such as boot-

strapping and monte carlo.

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MS39

Statistical Estimation and Identifiability of Dynamic Parameters in HIV/AIDS Dynamic Models

In this talk, I will discuss the issues of identifiability of dynamic parameters in differential equation models of HIV dynamics. We show that four parameters and the product of the remaining two parameters in the popular three dimensional HIV/AIDS model can be identified based on measurements of viral load. We propose a least square method to estimate the parameters without additional assumption about the initial condition. The proposed method is implemented to study the statistical identifiability of the dynamic parameters in simulation study and applied to virological response data from HIV-infected patients receiving antiretroviral treatment. A variety of statistical estimation methods for estimating the dynamic parameters in the differential equation models will be reviewed and discussed.

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MS40

Towards the Efficient Solution of Quantum Optimal Control Problems

Optimal control of finite-level quantum systems is discussed and a solution scheme for the optimization of a control representing lasers pulses is developed. The purpose of this external field is to channel the system's wavefunction between two given states in its most efficient way. This problem is solved numerically by multilevel iterative techniques. Some open issues regarding the solution of extended quantum optimal control problems are outlined.

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MS40

Electric Impedance Tomography with Circular Planar Graphs

We present an inversion method that handles the severe ill-posedness of Electric Impedance Tomography by proper sparse parametrization of the unknown conductivity. Specifically, we consider finite volume grids, which are resistor networks in disguise, with the resistors being averages of the conductivity over grid cells. We show that resistor networks can be recovered uniquely from Dirichlet-to-Neumann map measurements and thus can be used for estimating averages of the conductivity efficiently. Then we show how to incorporate a priori information about the solution.

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MS40

Distributed Parameter Identification for the FitzHugh-Nagumo Model of Electrocardiology

We consider distributed parameter identification problems for the FitzHugh-Nagumo system, aiming at reconstructing physical parameters from point electrical potential measurements over an interval of time. The inverse problem is posed as a PDE-constrained optimization problem, minimizing a regularized functional describing the mismatch between model prediction and measurement. We have developed a parallel algorithm of Newton-Krylov type, using PETSc. The method combines Newton's method for numerical optimization with Krylov subspace solvers for the resulting Karush-Kuhn-Tucker system.

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MS40

Multilevel Preconditioning Techniques for the Inversion of Convection-Diffusion-Reaction Equations and Incompressible Flows

We demonstrate multilevel preconditioning for the inversion of convection-diffusion-reaction (CDR) and the inversion of the initial state of an incompressible flow. The multi-level preconditioning is applied to the forward CDR operator in a reduced space sequential quadratic programming approach. In this case a simple velocity field is assumed. To extend this approach to a practical application, the velocity field should ideally be inverted. An example application could be the identification of chemical transport in an external flow where the velocity fields depends on weather dynamics. To this end we show that multi-level techniques designed for solving regularized ill-posed problems can be applied successfully to the inverse problem of reconstructing the initial state of an incompressible flow from sparse measurements in space and time. We show that, at fine resolution, this inverse problem can be solved at a cost that is a reasonably small multiple of the cost for a forward solve.

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MS41

Calculating Ion Permeation through Biological Channel Proteins

We have developed methodology to simulate the current of ions (Na+, Cl-, etc.) through a general three-dimensional ion channel structure embedded in a lipid bilayer when an electric potential is applied across the membrane. These calculations are done at the level of Brownian dynamics, i.e., ions are treated as particles and their motion is computed using a stochastic algorithm which simulates Brownian motion. Water solvent is treated as a dielectric continuum, which both supplies the thermal agitation underlying the motion of the ions and influences the electrostatic forces on these ions by virtue of its dielectric constant (which differs substantially from that of the protein-membrane complex). Application is made to the Glycine Receptor channel, emphasizing physico-chemical influences on ion current, e.g., charges of critical pore-lining amino acids, channel geometry, etc.

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MS41

Shockley-Ramo Theorem Allows a Glimpse Inside An Ion Channel

Theorems are rarely useful in biology but Shockley-Ramo SR* is an exception. This generalization of Kirchoff's current law relates measured macroscopic currents to atomic charge movements inside proteins. Such measurements of 'gating currents' are widely used to estimate energy of charge movements inside isolated proteins, even though isolated proteins do not exist in biology. Fortunately, SR supports general interpretations of gating current, although not every atomic model.*Nonner et al. Biophysical Journal 87: 3716 (2004).

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MS41

Poisson-Nernst-Planck Systems with Permanent Charges

We study Poisson-Nernst-Planck (PNP) systems with a piece-wise constant permanent charge as a model for ion flow through membrane channels. Assuming the ratio of the Debye length to the length of channel is small, we examine steady-states of boundary value problems of PNP systems using geometric singular perturbation approach. It turns out steady-state solutions exhibit two boundary layers at the two ends and two internal layers at each jump point of the permanent charge.

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MS41

Funneling Ions from Macroscopic to Atomic: Ion Access to Nanochannels

Ionic currents through protein channels of biological membranes depend on their atomic level structure and charge distribution of the proteins, but are driven by an applied electric potential and ion concentrations macroscopic distances from the channel. We analyze this multiscale problem with matched asymptotics, and demonstrate how the geometry of the access region controls ionic currents, giving new insights to the operation and design of channels as inherently multiscale nano-devices. Joint work with Bob Eisenberg, John Norbury, Zeev Schuss and David Holcman.

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MS42

Conformal Mapping of Some Non-harmonic Functions in Transport Theory

Since the nineteenth century, conformal mapping has been used to solve Laplace's equation by exploiting the connection between harmonic and analytic functions. In this talk, we note that another special property of Laplace's equation – its conformal invariance – is not unique, but rather is shared by certain systems of nonlinear equations, whose solutions have nothing to do with analytic functions. This simple observation leads to some unexpected applications of conformal mapping in physics. For example, it has generates a multitude of exact solutions to the Navier-Stokes equations of fluid mechanics and the Nernst-Planck equations of electrochemical transport. It also allows conformal-map dynamics for continuous and stochastic Laplacian growth (in models of viscous fingering and diffusion-limited aggregation, respectively) to be extended to non-Laplacian growth phenomena, such as advection-diffusion-limited aggregation (DLA in a fluid flow).

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MS42

The Average Shape of Transport Limited Aggregates

In this talk I will discuss the relation between stochastic and continuous transport-limited growth models. This study is based on a nonlinear integro-differential equation for the average shape of stochastic aggregates, whose mean-field approximation is the corresponding continuous equation. Focusing on the advection-diffusion-limited aggregation (ADLA) model, we show that the average shape of the stochastic growth is similar, but not identical, to the corresponding continuous dynamics. Similar results should apply to DLA, thus explaining the known discrepancies between average DLA shapes and viscous fingers in a channel geometry.

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MS42

Conformal Mapping Applied to New Engineering

Fluid Mechanics Problems

In this talk we shall discuss the application of conformal mapping to provide new insight into engineering problems, drawing on examples of inertially or viscously dominated flows. In the first instance, we shall discuss using conformal mapping the problem of how external straining flows affect the laminar wake signature of rigid bodies and lead to the surprising feature of vorticity annihilation and wake disappearance in multiphase flow problems. This leads to a justification for the wide spread assumption that viscous and inertial (inviscid) forces may be added together (which has previously been confirmed numerically) and how this affects the permanent flow signatures of high Reynolds number bubbles. In the second example, we show how using conformal mapping enables the significant body of research on viscous gravity currents to be naturally extended to when they are forced, either by an external ambient shearing flow or harmonic topography. Some of the results are confirmed using a physical analogue, in the spirit of Hele-Shaw's "magnetic field calculator". Finally, we will report some tentative new results on the use and application of conformal mapping to unsteady flow problems, an area which heither to has not received a great deal of attention.

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MS42

On a Class of Free-boundary Flows in Hele-Shaw Cell in the Presence of an External Field

Analysis of displacement of one fluid by another in a Hele-Shaw cell and porous media is a source of a multitude of mathematical problems which provide some insight into general features of nonlinear boundary dynamics. Here, we consider a slightly modified version of this classical problem. Generalized two-phase fluid flows in a Hele-Shaw cell are considered. It is assumed that the flow is driven by the fluid pressure gradient and an external potential field, for example, an electric field. Both the pressure field and the external field may have singularities in the flow domain. Therefore, combined action of these two fields brings into existence some new features, such as non-trivial equilibrium shapes of boundaries between the two fluids, which can be studied analytically. Some examples are presented. It is argued, that the approach and results may find some applications in the theory of fluids flow through porous media and microfluidic devices controlled by electric field.

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MS43

Light Trapping in Nonlinear Periodic Structures

An area of intense research is that of photonics, where light propagation features are controlled by clever engineering of periodic optical structures. For example, the fiber bragg grating where an additional intensity dependent nonlinear index of refraction allows soliton like propagation with tunable velocities. Here we consider nonlinear periodic geometries. We show that the additional transverse dimension allows for a richer dynamics of light trapping, bending and switching, provided stable gap soliton-like bullets exist.

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MS43

Nonlocal Stabilization of Ultra-short Pulses in Cubic Nonlinear Media

Abstract not available at time of publication.

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MS43

Solitary Waves in Discrete Media in the Presence of Four-wave Mixing Products

In this talk, I will discuss solutions that arise in a vector discrete model of the Nonlinear Schrodinger equation where nonlinear inter-component coupling and four-wave mixing are taken into account. We show that solutions to the equations give rise to both single and mixed mode branch solutions. Stability of these solutions is obtained by considering the so-called anti-continuum limit. We also connect this work with some recent experiments.

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MS43

Arrest of Collapse for the Nonlinear Schroedinger Equation by Dispersion-diffraction Management

Abstract not available at time of publication.

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MS44

Emerging Coherent Structures in the Dynamics of a Class of Nonlinearly Dispersive Evolution Equations

The interplay between nonlinearity and dispersion is thought to be responsible for solitary wave solutions of nonlinear dispersive equations. The exact mechanisms for which these waves emerge and dominate the long time asymptotics of a large class of initial conditions are not completely understood, especially in multidimensional settings. We study an equation class where the balance between dispersion and nonlinearity is varied continuously, which results in rich long time dynamical evolution. The family includes a special 1D case where the equation becomes completely integrable.

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MS44

Ultrashort Optical Pulses in Nanostructured Materials with Electric and Magnetic Resonance

Nanostructures embedded in a host material are capable of dramatically changing their optical properties. The most exotic property is negative refractive index, recently observed experimentally in the optical domain. This phenomenon results from simultaneous magnetic and electrical resonant interactions of nanostructures with an external electromagnetic field. We will analyze energy confinement and self-induced transparency phenomena both in the simplest case of metallic nanospheres and nonlinear dynamics of solitary waves in dual resonance materials. Ultrashort pulse dynamics will be analyzed for the case of bulk materials as well as for surface waves.

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MS44

Multi-dimensional Solitons in Nonlinear Wave Equations

Most solitions are one-dimensional waves, even in multidimensional equations. Solitons are nonlinear traveling waves where the nonlinearity and dispersion are balanced to create a stable coherent local environment so that that the solitions maintain their coherence when colliding with other solitions. Because the same dispersive operators are much stronger to two and three dimensions than in one dimension, this balance is usually lost when a one-dimensional equation is generalized to higher dimensions. We restore the balance by making the dispersion weaker in a class of KdV and regularized long wave equations to create fully two and three dimensional solutions.

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MS44

Emergence of Compact Patterns

Solitons, kinks or breathers, are manifestations of weakly nonlinear excitations which, for instance, arise in weakly anharmonic mass-particle chains. In strongly anharmonic chains the tails of the emerging patterns decay at a super-exponential rate. In the continuum limit the tail zone shrinks into a singularity where the nonlinear dispersion due to discreteness degenerates and the resulting solitary waves become strictly compact. Hence their name: compactons. We shall show how multidimensional compactons emergence and interact. Many of the compact patterns emerge in the continuum limit out of discrete dynamical systems (say, a chain of oscillators).

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MS45

Contact Network Epidemiology: Bond Percolation Applied to Infectious Disease Prediction and Control

In the early 20th century, two epidemiologists introduced a simple and powerful deterministic model for predicting infectious disease transmission which tracks the unidirectional movement of hosts among three states–susceptible (S), infected (I), and recovered (R). This *SIR* model provides important insight into the temporal progression of outbreaks and the efficacy of vaccination, and is the foundation for a recent proliferation in predictive methods. *Contact network epidemiology* is a particularly promising development in which bond percolation on random graphs is applied to modeling disease transmission through heterogeneous populations. I will discuss the generalization of the *SIR* model to disease propagation on graphs in which vertices and edges represent individual hosts and disease-causing contacts, respectively, and link recent theoretical results to issues of public health.

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MS45

Vaccination Strategies in a Realistic Social Network

We study the effect of different vaccination strategies on the spread of an epidemic on a network. The network is generated by an agent-based simulation of the city of Portland, OR. We compare a range of strategies: from as simple as a uniform vaccination campaign, where all people are equally likely to be vaccinated; to vaccinating those with the most contacts, to a strategy based on the PageRank that underlies Google's rankings. With increased sophistication comes increased benefit but also increased cost.

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MS45

A Likelihood Based Method for Simultaneous Real-time Estimation of R0 and the Serial Interval

The occurrence of new emerging infectious diseases require improved methods to quantify and understand their epidemiology. Ideally, such outbreaks should be rapidly classified so as to facilitate an appropriate and effective public health response. Unfortunately there are few, if any, available methods to effectively estimate these parameters rapidly and easily. We present a likelihood-based method for real time estimation of R0 and the serial interval using only daily case counts of the disease. The likelihood derived is a thinned Poisson. We describe how this can be considered an extension of a simple branching process. Simulations further reveal that the method is effective and accurate in estimating R0 when the serial interval is known and performs well when both R0 and the serial interval are estimated. Using data from the SARS outbreak in 2003, we illustrate the utility of this method and compare it with other estimates of these outbreaks.

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MS45

Spatial Epidemic Dynamics and Power-law Disease Transmission Models

The expected number of disease transmissions per day per infectious person during an epidemic has been found through high-fidelity agent-based simulation to scale approximately with the square of the susceptible fraction of the population. This is in contrast to the linear scaling assumed in traditional epidemiologic modeling. Treatment of the effects of the social contact structure through this power-law formulation leads to significantly lower predictions of final epidemic size than the traditional linear formulation.

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MS46

Efficient Shared-memory Algorithms and Implementations for Solving Large-scale Graph Problems

Graph abstractions are extensively used to understand and solve challenging computational problems in various scientific and engineering domains. They have particularly gained prominence in recent years for applications involving large-scale networks. In this talk, we present fast parallel algorithms for several large graph problems, on a variety of shared memory architectures. We first discuss the design and implementation of a large-scale graph theory benchmark, representative of computations in diverse disciplines such as computational biology and national security. We then present multithreaded algorithms for fundamental graph problems such as Breadth-First Search and st-connectivity. Based on these core graph algorithms, we have designed parallel implementations for the evaluation of widely-used centrality metrics in social network analysis (SNA). Using our algorithms, it is now possible to rigorously analyze networks three orders of magnitude larger than instances that can be handled by existing SNA packages. We highlight algorithm and architecture-specific optimizations to exploit properties typically observed in real-world large scale networks, such as the low average distance, high local density, and heavy-tailed power law degree distributions. We conclude the talk by presenting parallel performance results on large sparse-random synthetic graphs, as well as real datasets such as the web graph, protein-interaction networks, movie-actor and citation networks, on high-end shared memory symmetric multiprocessor and multithreaded architectures. We report near-linear speedup and high system efficiency for sparse graph instances with vertices and edges in the order of billions. This is a significant result in parallel computing, as prior implementations of parallel graph algorithms report very limited or no speedup on irregular and sparse graphs, when compared to the best sequential implementations.

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MS46

Massively Multithreaded Supercomputers for Discrete Mathematical Problems

We will discuss our experiences designing and using a software infrastructure for processing semantic graphs on massively multithreaded computers. We have developed implementations of several algorithms for connected components and subgraph isomorphism, and we will discuss their performance on the existing Cray MTA-2, and their predicted performance on the upcoming Cray Eldorado. We will also discuss our work with subgraph isomorphism heuristics. We will conclude with a discussion of other potential applications for these supercomputers.

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MS46

An Interactive Environment for Combinatorial Supercomputing

We describe a toolbox for combinatorial scientific computing that we are currently building in the framework of Star-P, which is a flexible interactive system intended to enable computational scientists and engineers to use a high-level language to program high-performance parallel supercomputers and commodity clusters. Our system includes distributed sparse array data structures and operations, which allow rather simple and elegant descriptions of various combinatorial and graph-theoretic computations. We have used it to explore graphs with hundreds of millions of vertices and billions of edges.

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MS46

Computational Methods for Detecting Network Vulnerability

Many types of systems are naturally modeled by networks, including the power grid, cyber security networks, and epidemiological networks. We will describe our work on computational techniques for high performance computing to detect network vulnerabilities where the network behavior is modeled with complex mathematical models. Our initial focus has been the electric power grid, where we try to detect small groups of lines that can cause a blackout when broken collectively; we generalize this to problems where the graph functioning is described by a complex mathematical model.

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MS46

Fast Shortest Path Computations on Large Networks

We present acceleration methods for shortest path computations on large networks. Our methods are based on Dijkstra's algorithm. We assume that for the same underlying network the shortest path problem has to be solved repeatedly for different node pairs. Thus, preprocessing of the network data is possible and can support the computations that follow. Our methods achieve speed-up factors of more than 1,500 on the German road network (5 million nodes, 12 million arcs).

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MS47

A Resource-based Model of Microbial Quiescence

Abstract not available at time of publication.

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MS47

Accounting for Asymmetries in Gender and Age-Specific Hiv Prevalence in Southern Africa

Young women in Southern Africa are three times more likely to be HIV infected than young men. The prevailing explanation for this is differences in the rates of transmission from male to female and female to male, however recent studies suggest this difference in transmission rates may not be present in Southern Africa. We use a gender- and age-structured model parametrized by South African census data to show that empirically derived asymmetries in sexual contacts can account for the differences in prevalence.

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MS47

Transmission Dynamics of Tuberculosis of Multiple Strains

Multiple-drug resistant tuberculosis (MDR-TB) and HIV co-infection of tuberculosis have created a serious worldwide challenge for the success of anti-TB control and elimination programs. In this talk, the transmission dynamics of tuberculosis is studied by a mathematical model that incorporates both exogenous re-infections of TB and drug-resistant strain and drug-sensitive strain of TB. The model presents several distinct bifurcations and multiple stable nontrivial steady states for both the basic reproductive number less than one and greater than one. A single tipping point (like the basic reproductive number) alone cannot determine the transmission dynamics. The full picture of the dynamics will be decided not only by parameters but also by the initial data. It also shows that MDR-TB can survival independent of drug-sensitive TB.

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MS47

Disease Transmission at Home and Abroad

Most simple disease transmission models assume well-mixed populations. Heterogeneities in transmission arising from age structure, behavioural groups, stages of infection and spatial variation are usually modelled by subdividing populations into well-mixed groups. In this talk I present a multi-group, multi-setting model for disease transmission and formulate conditions for disease spread. Different settings may include households, workplaces, transit or exciting after-hours establishments. Transmission is homogeneous within each setting, but not within each group.

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MS48

A Model Reduction Method for High-Dimensional Dynamical Systems

We present a computational technique for the reduction and analysis of a large class of coupled ODE systems, when the goal is to study the *fine structure* of multi-scale dynamics near known orbits. We demonstrate that a complex model can be reduced to a sequence of low-dimensional approximate models augmented by global consistency conditions. Small parameters in the system are *not* required, as estimation of relative scales in coupling terms and time scales are measured from the orbit in conjunction with the equations of motion. We illustrate the technique on several modelling examples and compare with other well-known techniques.

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MS48
Noise-Induced Phenomena in Slow-Fast Dynamical Systems

We consider slow-fast systems of coupled differential equations in which both slow and fast components are perturbed by white noise. Extending results from singular perturbation theory, we explicitly construct a neighbourhood of the slow manifold in which typical sample path concentrate. We also discuss the behaviour near bifurcation points, where noise may induce new phenomena such as stochastic resonance. Reference: N. Berglund, B. Gentz, Noise-Induced Phenomena in Slow-Fast Dynamical Systems. A Sample-Paths Approach. Springer, Probability and its Applications (2005)

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MS48
Computing Global Manifolds of Slow-Fast Systems

The presence of slow and fast variables in a model makes it very difficult to investigate the behavior numerically. It is already known that periodic orbits can be approximated very well in this context by using a two-point boundary value solver, e.g. AUTO. In this talk we explain how this idea can be taken further to compute global manifolds of periodic orbits. We will focus on one-dimensional manifolds in a Poincare section, but compare this with the corresponding two-dimensional manifolds in the full state space.

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MS48
Phase Response Curves, Delays and Synchronization

The phase response curve (PRC) of a periodically spiking neuron is a function that expresses the reaction of the neuron to small input pulses. We developed a new and very fast way to compute PRCs as a byproduct of a continuation algorithm. We found that delays can be crucial for the synchronizing abilities of networks of neurons through excitatory connections. Using the PRC of a neural model, one can compute the necessary delay to allow synchronization or phase locking.

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MS49
General Solutions of the Navier-Stokes equations in the Class of the Boussinesq-Rayleigh Series

In three dimensions, general solutions of the unsteady Navier-Stokes equations in the form of the Boussinesq-Rayleigh series are computed explicitly by symbolic programming and evaluated by parallel computing. We show that both forced flows and free-streams away from boundaries are nonlinear superpositions of the Stokes flow, the Bernoulli flow, the Couette flow and the Poiseuille flow. Emergence of multi-scale coherent structures is explained by existence of multi-valued general solutions for streamlines at high Reynolds numbers.

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MS49
General Solutions of Unsteady Stokes Equations

In the interest of producing differential representations similar to Papkovich-Neuber and Boussinesq-Galerkin, a general solution in terms of two scalar functions is produced for unsteady Stokes equations. New formulae connecting the differential representation and other solutions describing Stokes flows are provided. It is shown that the Lambs general solution follows by a suitable choice of the scalar functions. The unified approach presented here demonstrates an important link between oscillatory flows and flows through porous media.

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MS49
Slipping Stokes Flow around a Slightly Deformed Sphere

The resistance relations for a rigid, slightly deformed sphere in an unbounded Stokesian flow are generalized to the case where the surrounding fluid may slip at the surface of the particle. The resulting resistance formulas are found to be in perfect agreement with the numerical results for the slip-surface spheroidal particles, even in the case when deformations are not small. Further generalizations, like creeping thermophoretic and electrophoretic flows around slightly deformed sphere, are also addressed.

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MS50

MRA Based Limiting for Discontinuous Galerkin Methods

The discontinuous Galerkin (DG) method has established its importance in a wide variety of applications. The high-order DG method is ideally suited for problems in atmospheric science due to its inherent nature of being conservative and easy incorporation of monotonic limiters. Slope limiter is an important component of the DG method. These slope limiters have a problem dependent parameter which is chosen arbitrarily. An efficient way of estimating this parameter is yet to be designed for practical purposes. Due to the lack of a good limiter, which is problem independent and within the framework of conservation principle, application of this method to atmospheric problems is restrictive. It is no exaggeration to state that the design of a good and a robust limiter is a bottleneck to the development of DG method for solving conservation laws. We are working on building a limiter using multi-resolution analysis, which analyzes the solution structure at various scales.

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MS50

Multi-domain Multiresolution Based High Order Hybrid Methods for Hyperbolic Conservation Laws

We present the hybrid methods based on multi-domain and multiresolution analysis. For each sub-domain, a different high order method is adopted depending on the regularity of the approximation. In the first part, radial basis function method is discussed as a possible high order method adopted in the smooth regime. In the second part, we will present the Spectral-WENO hybrid method (SWHM). For the SWHM, the algorithm conjugates the non-oscillatory properties of the high order WENO scheme with the high computational efficiency and accuracy of spectral methods for nonlinear conservation laws in an adaptive multi-domain framework. A high order multi-resolution algorithm is used to adaptively keep the high gradients and discontinuities always inside a WENO subdomain to avoid the Gibbs phen onmenon while the smooth parts of the solution remain inside a Spectral one. We will discuss the treatment of the subdomain interfaces and the switching algorithm. One- and two-dimensional numerical examples will be shown.

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MS50

High-Order Discontinuous Galerkin Method for Problems with Shocks

Discontinuous Galerkin methods are a promising approach to high resolution computations of compressible flows with shocks in general domains. To resolve Gibbs phenomenon near discontinuities, a limiter is needed. We present a high-order limiter that is problem independent and parameter free. Adaptive computations can be very efficient in resolving fine solution features. We present space-time adaptive strategies with a method of lines and local accurate time stepping.

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MS50

Reconstructing a Discontinuous Function Using The Methods of Statistical Inference

By statistical inference I mean first, constructing a tractable statistical model of the functions to be processed, i.e. what sort of functions are common and what functions are rare. Then find the reconstruction algorithm (given some Fourier coefficients of a function) which has the smallest average error, with the average being over the statistical model. An infinite-dimensional gaussian model is used, modeling functions that are smooth everywhere except at a single, given point. We construct the optimal reconstruction process for this model, and demonstrate quite good performance. In addition we present a method for locating a jump discontinuity in an otherwise-smooth function, based on a slightly more complex statistical model. Numerical results are shown, with respectable performance, and we compare it to the jump locating algorithms of Gelb and Tadmor.

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MS51

Mesh Quality and Global Error Estimation in Anisotropic Fluid Flow Problems

In this talk we assess the impact of both anisotropic domains and anisotropic meshing on global error estimation problems, based on extrapolation coupled to the solution of adjoint problems for time integration. In particular we will assess the effectiveness of thge error estimates on simulation of chemical diffusion through "brick and mortar" like models of human skin.

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MS51

Measuring Anisotropic Behavior of Higher Order Derivatives for Mesh Adaptation

The error for piecewise polynomial interpolation is typically determined by the higher order derivatives of the approximated functions. We introduce some quantities to measure the anisotropic behavior of higher order derivatives in two and three space dimensions. We also describe how to estimate these quantities and how to use them for generating the nearly optimal anisotropic meshes.

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MS51

Mesh Quality and its Relationship to Linear System Solution Efficiency

Unstructured mesh quality signficantly affects the efficiency of the numerical solution of partial differential equations. This talk examines quantitatively the trade-offs between mesh quality improvement and solution efficiency. For simple finite element problems, we show the effect of mesh quality on the eigenvalue structure of the linear system and on solution efficiency. Also, for realistic finite element and finite volume application problems, we demonstrate that mesh improvement can significantly reduce overall time to solution.

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MS51

The Role of Mesh Quality in Theoretical Bounds for Finite Elements: A Survey

Mesh quality is critical for accuracy and efficiency in the numerical solution of partial differential equations. We will review theoretical bounds of the finite element analysis. Examples will include the analysis of interpolation error and of eigenvalue distribution of the stiffness matrix. We will emphasize the role of mesh quality in the theoretical bounds. Then we will discuss how these theoretical results can influence the design of mesh optimization algorithms.

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MS52

Methods for large-scale unconstrained optimization

Recent advances in large-scale constrained optimization have revived interest in methods based on sequential unconstrained optimization. Two methods for large-scale unconstrained optimization will be considered, each of which is based on the use of the preconditioned conjugate-gradient method. The first finds an approximate solution of a quadratically constrained trust-region problem. The second is a trust-search method that attempts to combine the best features of trust-region and line-search methods.

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MS52

Solution of Trust Region Subproblems by SSM

We present the local and global convergence properties of the Sequential Subspace Methods for minimizing a quadratic objective function over a sphere.

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MS52

The Return of the Filter Method

Filters are an alternative to penalty functions to promote global convergence in nonlinear optimization. A filter accepts a trial point whenever the objective or the constraint violation is improved. We present new filter active set approaches based on a two-phase methodology. Phase I estimates the optimal active set, and phase II performs a Newton step on the corresponding equality constrained problem. The approach allows inexact subsystem solves, making it suitable for large-scale optimization.

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MS52

Regularization and Trust Regions in Optimization

The trust region subproblem (the minimization of a quadratic objective subject to one quadratic constraint and denoted TRS) has many applications in diverse areas, e.g. function minimization, sequential quadratic programming, regularization, ridge regression, and discrete optimization. Recent advances in the theory and algorithmic development using Lanczos techniques have allowed TRS to be used to solve large scale optimization problems. We provide an overview of these new developments along with the relationships to Conjugate Gradient methods and regularization.

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MS53

Seven Deadly Sins of Modeling

It took over 30 years to move models and modeling from the mud room to the drawing room of American mathematics. With success has come a rather cavalier use of the word and the process. We will use examples to show how technology and our own emotions can lead us astray when we try to represent objects, processes or systems by mathematical constructs.

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MS53

What's Math Got to do With It?

Mathematics has acquired a number of stereotypes that may discourage even the most capable students from the major and prevent people in general from recognizing its permeation into almost everything else they value in life. In this talk, we face some of these stereotypes and consider whether they are justified. In so doing, we point out dozens of applications from pace-setting science to contemporary entertainment, from chart-topping business to national security, from leading-edge medicine to consumer products, where a good share of the excitement in the field is actually in the mathematics. We briefly learn to "read" a differential equation and consider how to map its solution onto a computer. Our goal is to show that mathematics is a vibrant field, worthy of study at the college level by majors and nonmajors alike. In fact, just as the English language is spoken by more people who are not native speakers than by natives, mathematics is used daily by more people who are not professional mathematicians than by professionals.

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MS53

Suggestions from the Real World About Improving Math Education

Because the goals and culture in business and industry in the United States are dramatically different from those in academia, the training that enables the mathematics professional to succeed in a nonacademic setting requires attention to skills that are not usually developed in the course of formal mathematical education. Using first-hand experience as a guide, this paper discusses some of the contrasts between the two environments, spotlights the ways in which the industrial applied mathematician contributes, and presents ideas for adapting mathematical training to serve the needs of graduates with industrial career aspirations. Recognizing the problems that currently exist in retaining students at all levels in mathematics courses, a number of suggestions are presented for improvement of mathematics curricula at all academic levels.

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MS53

Circles in Circles: Mathematical Modeling of Surface Water Waves

A raindrop strikes the surface of a puddle. A bomb strikes the surface of the ocean. Each impact creates concentric rings of waves moving outward from the center. How can we create a mathematical model of this situation? What insights can a mathematical model give? How can we be confident that the model is correct? What are the similarities and differences between the scales of raindrops or bombs?

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MS54

Adaptive Multiscale Stochastic Simulation of Biochemical Systems

The modeling and simulation of biological systems have attracted research interests from many different areas. Such systems may contain complex behaviors that are discrete, stochastic and multiscale. Stochastic simulation algorithms are often used in these studies. The SSA (Gillespie Algorithm) and the tau-leaping method are two of the most popular algorithms. Each of them works properly for problems in a certain scale. An adaptive algorithm that automatically chooses proper method for different problem scale is desired. In this talk we will introduce an adaptive algorithm that combines SSA and tau-leaping method to automatically choose the proper formula and stepsize to achieve high efficiency and accuracy.

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MS54

Spectral Methods for the Analysis of Stochastic Dynamical Systems

This talk presents our development of spectral methods for sensitivity analysis and reduced order modeling of stochastic dynamical systems that are governed by the chemical master equation. The sensitivity analysis relies on polynomial chaos expansions, which capture the nonlinear behavior of the system dynamics in response to finite-sized parametric perturbations. Reduced order models are obtained from Karhunen-Loève decompositions. We show applications of these methods to a bi-stable model system and a viral infection model.

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MS54

Metastability in Irreversible Diffusion Processes and Stochastic Resonance

During the last years, significant progress has been made in the quantitative description of metastability in reversible diffusion processes, whereas much less is known for irreversible diffusions. We consider the diffusion exit from a domain whose boundary is an unstable periodic orbit. Going beyond large-deviation results, we derive the distribution of the first-exit time explicitly, up to multiplicative errors in the prefactor. As an application, we shall discuss the phenomenon of stochastic resonance.

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MS54

Equation-Free Uncertainty Quantification on Stochastic Chemical Reactions

Equation-free (EF) methods have been used to accelerate fine-scale simulations and describe their coarse-grained evolution in dynamical systems where coarse equations may not be explicitly available. The methods have also been used, in the context of uncertainty quantification, to evolve projections of stochastic states, described by ODEs, onto generalized polynomial chaos (gPC) bases; this way the implementation of stochastic Galerkin projection codes could be circumvented. In atomistic models of chemical reactions one often does not have explicitly available coarse-grained chemical kinetic equations in terms of reactant concentrations; fine-scale algorithms (e.g. kinetic Monte Carlo) must be utilized to simulate reaction evolution. We combine the two approaches to study uncertainty quantificaton for stochastic models; this involves computing observables from the microsocpic simulator at three scales: the fine scale (reactant atom numbers), coarse-grained scale (reactant concentrations), and an even coarser scale (gPC projections of reactant concentration statistics). Random coarse-grained steady states can also be computed via this method. A stochastic model of a heterogeneous catalytic reaction, with mean species coverages as its coarse-grained observables, is used to illustrate this approach. The Gillespie stochastic simulation algorithm is used as the "inner" fine-scale simulator.

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MS55

Modeling Vortex Filaments with Stochastic Processes

Random vortex filaments are quite new objects and their theory is at the beginning. Nevertheless, they look promising for the purpose of describing turbulent fluids. We will focus on two main topics **(i) Description of vortex filaments using suitable stochastic processes and (ii) A limit behavior for a dense collection of vortex filaments**. The goal is to get some insight into behavior of turbulent flows.

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MS55

Stochastic Analysis and Simulation of Random Roughness in Shock Dynamics

We revisit the classical aerodynamics problem of supersonic flow past a wedge but subject to random roughness on the wedge surface. We first obtain analytical solutions for the inviscid flow with small random roughness on the wedge, and subsequently we perform stochastic simulations treating random roughness as a space-dependent random process. The results we present show that the high-order stochastic collocation method on a sparse grid can produce accurate results more efficiently.

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MS55

Adaptive Runge-Kutta Algorithms for Solving Folkker-Plank Associated Stochastic Differential Equations

Abstract not available at time of publication.

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MS55

Numerical Study of Interacting Particles Approximations for Integro-Differential Equations

Not available at time of publication.

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MS56

Predictive Capability of an HIV Model Calibrated with Treatment Interruption Data

We consider longitudinal clinical data for HIV patients undergoing treatment interruptions. Leveraging a statistically-based censored data method, together with inverse problem techniques, we estimate parameters in a biologically-based nonlinear dynamical model to fit each patient's data. The predictive ability of such a model is demonstrated by fitting it to half of each patient's longitudinal data, then using those estimated parameters to simulate the model over the full longitudinal time span. For many patients, the model accurately predicts the full longitudinal data set.

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MS56

Use of Antiretrovirals for Chemoprophylaxis and Therapy in Africa: New Opportunities, New Problems

Botswana has one of the highest rates of HIV infection in the world, with 37.4% of adults infected in 2003 according to UNAIDS. To address the problems of widespread infections, the government of Botswana instituted aggressive programs for the use of antiretroviral (ARV) drugs in both chemoprophylaxis for pregnant women and HAART therapy for treatment of clinical AIDS. At present, about 25% of AIDS patients receive HAART, and about 40% of HIV positive pregnant women receive chemoprophylaxis. After the country adopted an "opt out" policy for HIV testing in early 2005, these numbers are rapidly rising. Both the chemoprophylaxis regimen and the first line regimen for AIDS, include nevirapine (NVP). This is likely to cause problems with drug resistance when mothers with young infants need therapy, as about half of the mothers who receive NVP during labor reveal genotypic resistance when analyzed. In a recent trial we showed that NVP given only to newborn infants is as effective as when given to the mother during labor and the newborn infant, at least when used on a background of zidovudine (ZDV). This may provide a mechanism to avoid the establishment of NVP-resistance in HIV-positive mothers. HIV-1C, the subtype of southern Africa, shows higher rates of NVP-resistance as compared to HIV-1A or HIV-1D. Despite the potential for high levels of resistance, and advanced stages of disease, AIDS patients were very successfully treated with HAART. With initiation of drugs at median plasma viral loads of about 400,000 and median CD4 counts below 100, 87% of patients treated with ZDV + 3TC + NVP had undetectable RNA at 24 weeks after treatment, and 79% had undetectable RNA at 48 weeks. CD4 numbers increased by 149 at 24 weeks and 204 by 48 weeks. ZDV and 3TC containing regimens gave lower rates of viral resistance and less toxicity than regimens containing DDI and D4T.

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MS56

Backward Bifurcations in Disease Transmission Models

The first part of the talk will focus on designing models for assessing the theoretical impact of an imperfect HIV vaccine, which incorporate certain expected vaccine characteristics and HIV features, on HIV control. The second part addresses the issue of targeted use of anti-retroviral therapy and its impact on resistance development and transmission of resistant HIV.

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MS56

The Role of Transactional Sex in the Spread of HIV in Nigeria

The sex industry has been implicated in the spread of HIV across the world. In this article we study HIV transmission in one of the countries of sub-Saharan Africa, namely, Nigeria. We propose two models which describe the dynamic of HIV spread in Nigeria: the first one consisting of two core groups of high-risk sexually interacting heterosexual populations, and the second one with the two core groups linked to the general population. The core groups in the first model consist of male truck drivers and female sex workers. We obtain with our first model that the resulting sexual activities between truck drivers and sex workers are responsible for *fast* HIV/AIDS spread in these two groups. Moreover, these high-risk groups influence the disease spread in the general population and a simplified version of such dynamics is described in our second model. Thus, we explore the potential impact of high levels of infection in the core groups on the general population. One of the important consequences of this research is that we calculate potential results of prophylaxis.

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MS57

Modeling Circadian Rhythms in the Eye

In this talk, we present two mathematical models that deal with the photoreceptors in the eye. For the first model, we examine the interactions between the photoreceptors and the trophic pool and show that a stable limit cycle is predicted for a range of parameter values. It is known that the rods and cones undergo periodic shedding of their outer segments and we interpret this stable limit cycle as the mathematical description of an inherent circadian rhythm within the eye associated with the shedding process. For the second model, we describe the melatonin levels in the eyes and blood stream as limit cycle oscillators, thus assuming a priori the existence of a circadian rhythm. The modeling approach of the second model allows us to examine the proposed mechanisms for interaction. We conclude that a simple diffusive process describing the flow of melatonin between the eyes is not sufficient to describe observed experimental results.

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MS57

The Stochastic Beverton-Holt Equation

In the Beverton-Holt difference equation of population biology with intrinsic growth parameter above its critical value, any initial non- zero population will approach an asymptotically stable fixed point, the carrying capacity of the environment. When this carrying capacity is allowed to vary periodically it is known that there is a globally asymptotically stable periodic solution and the average of the state variable along this solution is strictly less than the average of the carrying capacities, i.e. the varying environment has a deleterious effect on the state average. In this work we consider the case of a randomly varying environment and show that there is a unique invariant density to which all other density distributions on the state variable converge. Furthermore, for every initial non-zero state variable and almost all random sequences of carrying capacities, the average of the state variable along an orbit and the average of the carrying capacities exist and the former is strictly less than the latter.

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MS57

Multiple Rhythms of the Nervous System

The nervous system produces many different rhythms, some simultaneously, in different behavioral situations. This talk focuses on the rhythms of the entorhinal cortex (EC), the gateway of the hippocampus. The talk discusses the gamma (40-90 Hz), theta (4-12 Hz) and beta1 (13-20 Hz) frequency bands, and how they interact, using low dimensional maps to describe central features of the dynamical behavior.

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MS57

Mathematical Models of Tumor-immune Interactions: Desigining Effective Immunotherapy Protocols

Cancer is a myriad of individual diseases, with the common feature that an individual's own cells have become malignant. It is believed that a healthy individual keeps potentially cancerous cells from developing into a threatening tumor through a complicated network of immune responses and mechanisms built into the cell cycle that recognize aberrant cells and control their proliferation. Thus, the treatment of cancer poses great challenges, since an attack must be mounted against cells that are nearly identical to normal cells. In particular, chemotherapy has had limited success due to the toxicity of most treatments to many cells that are crucial to the normal functioning of the patient. Therefore, much attention has recently been focused on immunotherapy, i.e. methods of strengthening the patient's own immune response to cancerous cells. Mathematical models of tumor growth in tissue, the immune response, and the administration of immunotherapy can suggest treatment strategies that optimize treatment efficacy and minimize negative side-effects, such as an autoimmune response. In this talk we will present our work in this area over the last five years, highlighting both the successes and the remaining challenges.

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MS58

Temporal and Spatial Adaptivity in High-order Discontinuous Galerkin Particle-in-cell Methods

We discuss the continued development of a high-order particle in-cell method. The high-order method uses fewer grid points to resolve plasma dynamics as compared to classical finite difference methods while using a boundary fitted unstructured grid. We discuss implicit-explicit Runge-Kutta schemes that enhance temporal flexibility. We also discuss adaptive particle deposition techniques to enhance geometrical flexibility.

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MS58

Adaptive Dual Particle Solid Impact Simulations

We will discuss the recent developments of the Dual Particle method. We will cover three issues. 1) We will discuss the fundamental idea and properties of the method 2) We will discuss the option of adapting particles using methods previously developed for particle methods and adapted to the dual particle description where two different sets of aprticles are used for different quantities 3) We will discuss specific applications of the method

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MS58
AMR-PIC Modeling of Plasmas and Beams

Modeling of systems that involve a wide range of scales in space and/or time is challenging. We present emerging techniques for modeling plasmas and beams, based on the Particle-In-Cell (PIC) and Adaptive Mesh Refinement (AMR) methods. The coupling of these two well-known methods must be done with care in order to avoid unwanted effects (spurious self-forces, reflections patch boundaries, ...). We will present the main issues, solutions and examples of application to particle beam modeling and laser-plasma interaction.

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MS58
Particle-in-cell Method for Fluid-Structure Interactions

The particle-in-cell method possesses advantages of both Eulerian and Lagrangian methods while avoids their difficulties. Recently we combined the particle-in-cell method with newly developed two-phase flow theory to study fluid-structure interactions. The fluid and the solid structure are treated as two continuous phases in the two-phase flow theory. In this presentation, we outline basic principles of the two-phase flow theory and numerical schemes of the particle-in-cell method and then provide examples of their applications.

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MS59
Optimal Vaccination Strategies for the Control of Rabies among Raccoons

We seek the best vaccination strategy to control the spread of rabies among several subpopulations of raccoons. We construct a metapopulation SIR model with control functions, the rate of vaccination in each subpopulation. Transition rates between subpopulations are assumed to depend on the spatial distance between subpopulations and disease status.

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MS59
Optimal Harvesting of a Semilinear Elliptic Fishery Model

We are considering an optimal harvesting problem for a semilinear elliptic fishery model, which has logistic growth and the harvest depends on the location of the fish. We seek to maximize the yield while minimizing the cost[1] and variation[2] of the fishing effort. Existence, necessary conditions and uniqueness for the optimal harvesting control are established. The optimal pattern for 2 is characterized by a variational inequality involving the solutions of an optimality system of nonlinear elliptic partial differential equations. Numerical examples are given to illustrate results.

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MS59
Optimal Harvesting in An Age-Structured Predator-Prey Model

We investigate optimal harvesting control in a predator-prey model in which the prey population is represented by a first order partial differential equation with age-structure and the predator population is represented by an ordinary differential equation in time. The controls are the proportions of the populations to be harvested, and the objective functional represents the profit from harvesting. The existence and uniqueness of the optimal control pair are established.

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MS59
Optimal Harvesting During an Invasion of a Sub-

lethal Plant Pathogen

Plant pathogens are quite destructive to cash crops throughout the world resulting in potentially devastating financial losses. This work expands recently developed optimal control theory for an integrodifference model to a mathematical system which includes an integrodifference component. This system models a highly simplified plant pathogen system for which the optimal harvesting scheme is derived. An adjoint system is introduced to characterize the optimal harvesting pattern. This analysis shows that while it may not be possible to prevent losses upon discovery of the pathogen in an area, it is theoretically possible to significantly cut those losses by culling an area around the initial infection.

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MS60

Culture and Environment as Determinants of Women's Participation in Computing

This talk presents a cultural perspective towards thinking about, and acting on, issues concerning women and computer science and related fields. We posit and demonstrate that the notion of a gender divide in how men and women relate to computing, traditionally attributed to gender differences, is actually a result of cultural and environmental conditions. Indeed, the reasons for women entering - or not entering - the field of computer science have little to do with gender and a lot to do with environment and culture as well as the perception of the field. Appropriate outreach, education and interventions in the micro-culture can have broad impact, increasing participation in computing and creating environments where both men and women can flourish. This argument is illustrated by specific case studies.

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MS60

Enhancing Diversity in the Mathematical Sciences: A View from Educational Research

In order to understand the obstacles women and underrepresented minorities face in science and mathematics, and possible supports to them as they work to overcome those obstacles, we need to begin with the question of what it takes to succeed in these fields. Theories of situated learning posit that learning happens through participation in social practices, and that learning is inseparable from that participation. Students learn from what they do, and the activities in which they engage determine the particular things they learn. Each set of activities-for example, listening to teacher explanations, completing various types of homework and in-class exercises, taking notes, working with other students to solve problems, reading texts, studying for and taking exams, attending seminars and conferences-constitutes a different type of learning opportunity. Inherent in this perspective is the idea that learning mathematics is actually a three-dimensional process, involving the acquisition of mathematical content, participation in mathematical practices, and developing an identity as a mathematics learner. Participation and developing an identity are particularly challenging for women and students of color, who are often excluded from important mathematical practices and receive a variety of messages about ways that they do not belong. I will talk about a variety of strategies that have been proven successful in minimizing these challenges, providing equal opportunities for all students to engage in and contribute to the mathematical sciences.

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MS60

Increasing the Number of Minority Ph.D.'s in Mathematics

Over twenty percent of the graduate students in Mathematics at the University of Iowa are US minorities from groups underrepresented in Mathematics. Last year three US minority students earned Ph.D. s in Mathematics at Iowa, approximately ten percent of the total nationally. In 2005 the Department received the Presidential Award for Excellence in Science, Mathematics and Engineering Mentoring for its work toward increasing the number of US minority Ph.D. s in Mathematics. In this talk I will discuss our efforts toward this end. These efforts include the building and fostering of community, intensive mentoring by both faculty and peers, and the identification and nurturing of previously untapped talent. I will also discuss our efforts to institutionalize the changes that we have made. Finally I will discuss the replicability of our program. Throughout I will emphasize the benefits that accrue to all students.

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MS60

Successes and Challenges in Diversifying Research Universities and the National Science and Engineering Workforce

The speaker will focus on the general challenges that the country faces today concerning increasing the representation of those groups that have been traditionally underrepresented in mathematics, science, and engineering. He will share relevant formative experiences encountered along his life's journey as a publically educated first generation Mexican American from the barrios of Los Angeles to a Rice University Mathematics Professor and a President Clinton appointee to the National Science Board. As the Director of the Rice mathematical and engineering sciences program, a program well recognized for its production of minority PhD's, he will describe challenges, successes, and lessons learned along the way. Particular attention will be paid to the role of mathematics and mathematicians.

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MS61

Nonlinear Fokker-Planck Equations coupled with Navier-Sokes Equations

I will discuss the regularity and asymptotic behavior of nonlinear Fokker-Planck equations coupled with Navier-Stokes equations.

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MS61

Transport and collective dynamics in suspensions of swimming particles

This talk describes very recent work motivated by observations that populations of swimming bacteria exhibit a fascinating variety of phenomena including regimes of anomalous transport as well as spatiotemporally coherent fluid motion on scales much larger than the organisms. We propose a simple model of a swimming organism that is amenable to direct simulations of large populations. Hydrodynamic coupling between the swimmers leads to coherent motions in the flow that are consistent with experimental observations. At low concentrations, swimmers propelled from behind (like spermatazoa) strongly migrate toward solid surfaces in agreement with simple theoretical considerations; at higher concentrations this localization is disrupted by the coherent motions. Correspondingly, at large concentrations the swimmers move with velocities significantly larger than they could achieve in isolation.

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MS61

Mathematical Analysis of Certain Analytic Subgrid Scale Models of Turbulence

In this talk I will discuss the mathematical difficulty in proving global regularity for the three-dimensional Navier-Stokes equations. Furthermore, I will show the global regularity for certain analytic three-dimensional sub-grid scale models of turbulence. This will include the Smagorinsky model, Navier–Stokes-alpha model, the Leray-alpha model, the modified Leray-alpha and the Clark-alpha model. All these models are of nonlinear parabolic type and each has a finite dimensional global attractor. In some cases I will provide explicit bounds for the fractal and Hausdorff dimensions of these attractors, in terms of the relevant physical parameters. In addition, I will also prove the global regularity for the "shell model" of turbulence and show that it has a finite dimensional inertial manifold. Hence, this model can be reduced to a finite dimensional ordinary differential system. As a result, one can show that this model has a unique invariant measure associated with its dynamics when it is kicked randomly.

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MS61

Nematic Polymers Under External Fields

In this talk I will discuss new theoretical developments in the study of nematic polymers in the presence of external fields.

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MS62

Reducing Computational Cost in Simulation-Based Optimization

We examine a number of approaches to reducing the cost of design optimization, where the cost is due to the expense of contributing simulations or to the complexity of the underlying problem or to the need to include uncertainties in the design problem formulation. The approaches under investigation include the use of variable-fidelity models, distributed optimization algorithms, and variable reduction. We investigate comparative analytical and computational properties of the methods in application to aerospace problems.

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MS62

Uncertainty Affected Control Via Convex Programming

Solving discrete time finite/infinite horizon linear dynamic systems, under additional state-control resstrictions, leads to an intractable nonconvex optimization problem. We introduce a reparametrization scheme using "purified outputs" and show that the state-control trajectory becomes an affine function in the design variables as well as in the uncertain parameters of the system. Consequently,the task of synthesizing a constrained robust controler reduces to solving an explicit convex programming problem.

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MS62

High Performance Computing for Constrained Optimization with Application to Optimal Design and Control of a Racing Yacht in the America's Cup

We consider the analysis and development of robust and efficient optimization algorithms for the optimal design and control of a racing yacht in the America's Cup. The main emphasize is put on the optimal design of the hull-keel-winglet configuration as well as model reduction toward real time control of the boat. The considered optimization problems involve very large and highly coupled system of

PDE constraints. In that context we address more specifically the following issues:

- Adaptivity for time dependent optimal control problem
- Parallel processing for PDE constrained optimization problem
- Parameter identification problem toward model reduction
- Sensitivity analysis and optimal experiment design

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MS62

Numerical Optimal Control of the Wave Equation: Optimal Boundary Control of a String to a Prescribed State in Finite Time

In many real-life applications of PDE constrained optimization, hyperbolic equations are involved. Because of their possibly nonsmooth behaviour they constitute a severe challenge to both theory and numerics of those problems. In the present paper, optimal control problems for the well-known wave equation are investigated. The numerical method chosen here is a full discretization method based on appropriate finite differences by which the PDE constrained optimal control problem is transformed into a nonlinear programming problem (NLP). The intention is to study the order of the numerical approximations for the optimal control variables. Hence we follow the approach "first discretize, then optimize", which allows us not only to make use of the powerful NLP methods, but also to compute sensitivity differentials, a necessary tool for real-time control.

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MS63

Splitting Methods For Linear Separable Partial Differential Equations And Beyond

Splitting methods are numerical integrators for solving differential equations which are separable in solvable parts. The Schrdinger and Maxwell equations are relevant examples in physics and engineering of separable PDEs, and a large number of splitting methods from the literature can be used. However, the structure of these linear separable PDEs allowed us to build for them new tailored methods which outperform the known methods. Their performances will be tested on the Schrdinger equation.

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MS63

Forward Time-Step Splitting Methods For Solving Physical Evolution Equations

The solution of many physical evolution equations can be expressed as an exponential of two or more operators acting on initial data. Accurate solutions can be systematically derived by decomposing the exponential in a product form. This is the general splitting method of solving evolution equations. For time-reversible equations, it is immaterial whether or not the split coefficients are positive. On the other hand, most symplectic algorithms for solving classical dynamics contain some negative coefficients. It is only recently that the forward splitting algorithms are recognized as a highly effective in solving BOTH time-reversible and time-irreversible equations. This talk will summarize the basic structure applications of the forward splitting algorithms for solving diverse physical evolution equations.

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MS63

Description Of Light Focusing By A Lens Using Integral Solutions Of The Wave Propagation Equation

An accurate description of light focusing by even a simple single element optic, such as a spherical lens, is computationally quite challenging because of the need to evaluate multiple (typically quadruple) integrals having very highly oscillating integrands. The integrals arise from the diffraction theory of Stratton and Chu, which applies the vector form of Green's theorem to determine the electromagnetic fields at a point inside a closed volume in terms of the values of the fields known on a curved surface. Applying the theory successively to the two curved surfaces that constitute a lens we obtain the values of all the electromagnetic field components outside the lens in integral forms. We demonstrate how the integrals can be evaluated using current computational resources, including the splitting method, for high speed commercial lenses.

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MS63

Stability And Convergence Of The Adaptive Splitting Methods For Certain Singular Problems

We will focus on a split cosine scheme for a nonlinear solitary wave equation in two dimensions which arises in rectangular large-area Josephson junctions. The semi-discretization approach leads to a system of asymptotically separable second-order nonlinear ordinary differential equations. The numerical solution of the system is obtained via a further application of a linearly implicit splitting method. This yields, however, a concern of the numerical/computational stability and convergence. In this talk, rigorous analyses will be outlined on the stability, asymptotic stability and convergence of the numerical method.

Further discussions will be proposed.

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MS64

Fast Direct Solvers for Integral Equations

In this talk we consider the design of fast direct solvers for integral equations that exploit the Fast Multi-pole Method (FMM) structure of the matrix. The idea is to see if we can design solvers that are faster than the Hierarchically Semi-separable (HSS) fast direct solvers.

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MS64

Moore-Penrose Inversion of Hierarchical Semi-Separable Systems

The Hierarchical Semi Separable (HSS) matrices of low degree form an interesting class of (weakly) structured systems originally introduced by Shiv Chandrasekaran and Ming Gu. The class is closed under a number of numerical operations such as LU-factorization, matrix inversion (when the matrix is invertible), and Cholesky factorization (when the matrix is positive definite). The new result that will be presented in this talk is that it is also closed for URV factorization and Moore-Penrose inversion. A number of further properties will also be touched at, such as formal representations of HSS systems, the connection between the HSS structure and the classical quasi-separable or time-varying structure (sometimes called 'SSS' for Sequentially Semi-Separable), and model reduction for HSS systems. The latter theory may be of paramount importance in the quest for adequate pre-conditioners for large systems of equations, probably the most important application of HSS systems.

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MS64

Schur-Monotonic Semi-separable Matrix Approximations to SPD Matrices

Given a symmetric positive definite matrix A, we develop a fast and backward stable algorithm to approximate A by a symmetric semi-separable matrix to any given tolerance. We embed our approximation scheme inside a Cholesky factorization procedure to ensure that each Schur complement during the factorization remains symmetric positive definite after approximation. This, in turn, guarantees that the symmetric semi-seperable matrix approximation remains positive definite for any given tolerance. Numerical results will be provided and implications of this work will be discussed. Joint work with S. Chanderasekaran, X.S. Li and P. Vassilevski

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MS64

Large Rank Structured Matrix Computations using the Givens-weight Representation

In this talk we will show how several matrix computations involving rank structured matrices can be performed efficiently and accurately when the Givens-weight representation is used.

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MS65

Modeling Spatial Dynamics of Influenza Spread Using Traditional and Nontraditional Surveillance Data

There is surprisingly little empirical evidence on how influenza spreads through cities, regions, nations and across the globe. Documenting spatial patterns of influenza epidemics represents a first step toward understanding underlying mechanisms that drive epidemic fluctuations, and will help with the evaluation of targeted pandemic control strategies. Using novel and traditional influenza surveillance datasets, we have developed models of influenza spread that provide evidence to support control strategies at both the national and local scales. First, we model national spread of the yearly influenza epidemics so as to understand the impact of multivariate factors that drive large-scale spread, including population movement and environmental conditions. Second, we develop spatial models of local influenza spread across major metropolitan areas using real-time surveillance to define important demographic risk factors. Our research highlights the role of empirically-based spatial models to identify factors that are key in disease spread and for which targeting of control strategies may help stem the spread of pandemic influenza.

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MS65

Planning for Pandemic Influenza: Hospital Bed Surge Capacity Analysis for Los Angeles

The continued threat of the emergence of an influenza pandemic poses a significant global challenge. In order to minimize the effects of a pandemic, the health care system must be prepared to cope with mass illness and the burden on the health care services. As many uncertainties are involved in this type of studies, I will describe and compare different scenarios to understand the potential impact of a pandemic on hospital admissions in five counties in California. Our analyses show that results based on aggregated hospital resources can underestimate the true capacity at local hospitals.

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MS65

Resonance and the Seasonality of Influenza Epidemics

Influenza incidence exhibits strong seasonal fluctuations in temperate regions throughout the world, concentrating the mortality and morbidity burden of the disease into a few months each year. The cause of influenzas seasonality has remained elusive. Here we show that the large oscillations in incidence may be caused by undetectably small seasonal changes in the influenza transmission rate that are amplified by dynamical resonance.

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MS65

On the Role of Cross-Immunity and Vaccines on the Survival of Less Fit Flu-strains

A pathogen's route to survival involves various mechanisms including their ability to invade (host's susceptibility) and their reproductive success within an invaded host ("infectiousness"). The immunological history of an individual often plays an important role in reducing host's susceptibility or it helps the host mount a faster immunological response de facto reducing infectiousness. The cross-immunity generated by prior infections to influenza A strains from the same subtype provide a significant example. In this paper, we study the role of invasion mediated cross-immunity in a population where a precursor related strain (within the same subtype) has already become established. An uncertainty and sensitivity analysis is carried out on the ability of the invading strain to survive for given cross-immunity levels. Our findings indicate that it is possible (for relative low levels of cross-immunity) to increase the likelihood of strain coexistence even in the case when invading strains are "unfit", that is, when the basic reproductive number of the invading strain is less than one. The development of "flu" vaccines that *minimally* enhance herd cross-immunity levels may, by increasing genotype diversity, help facilitate the generation and survival of novel "virulent" strains, that is strains that have high levels of reproduction within the host.

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MS66

Single Frequency Characterization of Complex Targets in Remote Sensing

A new class of monochromatic target imaging and characterization algorithms for remote sensing has been developed which overcomes many of the traditionally encountered limitations, and artifacts such as so-called multipath returns, resulting from high frequency approximation-based backscattering techniques. We will demonstrate that given, either high or low, fixed-frequency monostatic radar data over one period of a tumbling object, that robust and efficient automatic characterization of complex non-convex, e.g. targets with open ports or cavities, is possible.

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MS66

Correlating Sensor Tracks with the Deterministic Annealing Method

Surveillance systems often involve multiple sensors tracking multiple objects. To maximize the preservation of information gained by each sensor a mapping must be performed between the objects in each sensors field of view. Due to differing sensitivity and geometry the number of objects detected by each sensor might not be the same. Object correlation is further complicated because there tends to be sensor bias due to pointing errors. This talk discusses the deterministic annealing approach to object correlation and sensor bias removal.

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MS66

Feature Extraction For Classification: Class Independent Statistics vs. Class Specific Statistics

There currently exist a large number of algorithms aimed at reducing the dimensionality of a feature set used for classification by relying on the statistical properties of the underlying distribution of data. Three common and well known examples of this type of technique are Principle Component Analysis (PCA), Multiple Discriminant Analysis (MDA) also known as Linear Discriminant Analysis (LDA), and Singular Value Decomposition (SVD). Each technique has its own operating conditions and a priori assumptions about the statistical nature of the data. In particular, for classification, of the techniques mentioned, only the MDA algorithm explicitly uses class information. Recently there has been interest in comparing PCA against MDA [?]. It is generally felt that the projected feature subset produced by MDA is better for classification purposes since the MDA algorithm finds a linear transformation that maximizes a measure of class separation. In this paper we will empirically compare and contrast the performance of the PCA, MDA, and SVD techniques on a variety of standard data sets. In addition, we introduce two additional algorithms called Classwise Principle Component Analysis (C-PCA) and Classwise Singular Value Decomposition (C-SVD), based on PCA and SVD respectively, that incorporate class-specific information into their constructions. We will demonstrate empirically that these new algorithms classify data better than their standard PCA and SVD counterparts. In addition to classification, each of the algorithms we present has a natural method for dimensionality reduction via eigenspace truncation. As such, we will also present results examining how classification performance degrades as the number of implicit algorithm-specific degrees of freedom are decreased. Our results demonstrate that the C-PCA and C-SVD techniques allow one to potentially do significant dimensionality reduction with negligible impact in classification accuracy.

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MS66

A Method for Sensor Management with Information Theoretic Objectives

Sensor management is a stochastic control problem in which the objective is to maximize accuracy in an underlying estimation task. While the optimal solution can be formulated as a dynamic program, its solution generally requires intractable computation and storage. We describe a heuristic method, motivated by results from submodular optimization, to a problem in which estimation performance is measured by conditional entropy. We explore bounds that can be obtained on the performance of the algorithm.

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MS67

A Fully Implicit Hall MHD Algorithm in 3D

We present a fully implicit, nonlinear algorithm for Hall magnetohydrodynamics (HMHD). HMHD supports dispersive waves ($\omega \sim k^2$), which result in explicit CFL conditions $\Delta t \sim \Delta x^2$. This precludes the use of explicit algorithms. Implicit methods can in principle step over such fast time scales, but the spectral properties of the associated matrices break most iterative methods. Here, we demonstrate a successful, scalable implicit solver based on physics-based preconditioned Jacobian-free Newton-Krylov methods.

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MS67

Domain Decomposed Implicit Methods for Model Magnetohydrodynamics Problems

We discuss domain decomposed, fully coupled, fully implicit solutions for time dependent magnetohydrodynamics models. Our current approach uses high order temporal discretizations and Newton-Krylov-Schwarz methods, where nonlinear Newton iterations are combined with additive Schwartz preconditioned Krylov subspace iterative linear solvers. We consider algorithmic and implementation issues related to the Schwartz preconditioning technique for problems with Dirichlet and periodic boundary conditions. Performance of one- and two-level algorithms with LU or ILU solves on subdomains is investigated and parallel convergence results are reported.

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MS67

An Implicit Method for Magnetic Fusion Mhd Calculations Using Adaptive, High-Order, High-Continuity Finite Elements

Many aspects of the physics of toroidal magnetic fusion experiments can be described by a set of "Extended Magnetohydrodynamic" (E-MHD) equations for the evolution of the fluid-like quantities describing the high-temperature plasma and the magnetic field. Because of the multiplicity of time and space scales that develop, it is now recognized that adaptive higher-order finite elements with an implicit time integration scheme offer significant advantages. An ongoing effort to solve these E-MHD equations with elements with C^1 continuity is described. This leads to a compact representation and efficient solution algorithm. The method builds on a formalism for representing the velocity in a potential/stream-function form, and the magnetic field in an intrinsically divergence-free form. Recent applications and future directions will be discussed.

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MS67

Preconditioning Implicit Simulations of Resistive Fusion Plasmas

Computational MHD poses challenges due to its wide range of spatio-temporal scales, strong anisotropy and nonlinearity. Additionally, resistive MHD experiences increased ill-conditioning as the spatial meshes are refined to resolve diffusive layers. We consider preconditioning techniques for these effects in the linear implicit system, based on optimized solvers for a decomposition of the system into individual sub-systems. We demonstrate that such an approach grows increasingly necessary for efficient solution strategies as the spatial mesh is refined.

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MS68

Rapid Development of Efficient Codes for PDE Simulation and PDE-Constrained Optimization

Abstract not available at time of publication.

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MS68

Single-Phase Groundwater Flow Simulation Using Sundance

We consider a nonlinear model for flow in porous media, with particular focus on the nonlinear advective acceleration term. Other macroscale models assume advective acceleration provides negligible contribution to momentum balance and excluded it in simulations. This assumption hinges upon the generally slow flow of groundwater. No one has investigated the "significance" of advective acceleration for intermediate Reynolds numbers, particularly for heterogeneous media. In this talk we provide our definition of "significant", and numerical results from two- and three-dimensional single-phase flow which categorize the importance of advective acceleration.

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MS68

NEWCON: Nonlinear Model Predictive Control Package

This talk describes the development of NEWCON, a model predictive controller package. The Newton-type control law formulation, based on works of Oliveira (1994) and Santos et. al. (1995) is solved using a multiple shooting approach and sequential quadratic programming. High quality numerical packages CVODES and HQP are used for the integration and sensitivity analysis of the system model and for the solution of the resulting optimization problem, respectively.

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MS68

Large Scale Data Assimilation for Atmospheric Chemical Observations

The task of providing an optimal analysis of the state of the atmosphere requires the development of novel computational tools that facilitate an efficient integration of observational data into models. We discuss several new computational tools developed for the assimilation of chemical data into atmospheric models. They include automatic code generation of chemical adjoints, properties of adjoints for advection numerical schemes, calculation of energy singular vectors and their use in placing adaptive observations. Data assimilation results using both variational and ensemble based methods are shown for several real test problems to illustrate the power of the proposed methods.

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MS69

Space-Time Response of Nematic Polymers in Small-Amplitude Oscillatory Flows

The space-time responses of nematic polymers to the small-amplitude oscillatory shear flows have been studied using a mesoscopic model which incorporates a coupling between short-range excluded volume interactions, anisotropic distortional elasticity. The analytical solutions of the nematodynamic equations are obtained at small amplitudes. The external frequencies bring new length scales for both the velocity and orientation structures. The velocity and the director angle show boundary layers with thickness proportional to $\frac{1}{\sqrt{Er\omega}}$ in both low and high frequency cases at the first order while the order parameters show at the second order with boundary thickness proportional to $\frac{1}{\sqrt{Er\omega}}$ or

$\frac{1}{\sqrt{Er}}$ and show a frequency precession with that of the velocity and the director angle. The molecular shape parameter will change a molecular direction when the molecule shifts from a flow-aligning regime to tumbling regime. The steady state structures in weak shear and Poiseuille flows are recovered with no boundary layers in the frequency limit $\omega = 0$. The storage and loss moduli have been calculated.

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MS69

Dynamics of Magnetic Dispersions in Simple Flows Modelled By Kinetic Theories

We establish the reciprocity principle of the Doi-Hess kinetic theory for rigid rod macromolecular suspensions governed by the strong coupling between an excluded volume potential, linear flow and a magnetic field. The principle provides a reduction of the Fokkar-Plank equation from a 5-parameter to a 2-parameter family of coplanar linear flows and magnetic fields. The planar flow with a rotational component maps to a simple shear with a transverse magnetic field. Here we predict the transition phenomena associated with each robust class of sheared monodomain attractors, as the magnetic field is turned on and magnified. The irrotational flow reduces to a pure extension subject to a transverse magnetic field. The equilibrium solution is of the Boltzmann type, parameterized by a pair of order parameters and the resulting PDF generically biaxial.

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MS69

Nonlinear Viscoelasticity and Finite Depth Effects in the Ferry Shear Wave Experiment

We revisit the classical oscillatory shear wave experiment and model of Ferry and collaborators, motivated by viscoelastic characterization experiments on lung airway surface liquids (ASLs). We first extend the classical model and solution to finite depth, and estimate errors in inverse characterization of storage and loss moduli due to application of the Ferry semi-infinite formulas. We identify regions in storage-loss moduli space where finite depth effects are minimal, yet other regions where application of the Ferry formulas lead to enormous relative errors. We focus these evaluations at frequencies of plate oscillation and imposed bulk strains that are representative of biological conditions on ASLs. Next, we consider a fundamental biological question: are nonlinear material properties exploited under typical *in vivo* conditions? For ASLs, coordinated cilia as well as tidal breathing cycles induce finite oscillatory shear strains; we model these conditions by studying shear wave and stress features versus imposed bulk strain. We sacrifice the complex modulus function $G^*(\omega)$ in favor of nonlinear constitutive laws of Maxwell and Giesekus type, using $G'(\omega)$ and $G''(\omega)$ at plate frequency ω to define the Maxwell model parameters. A quasilinear model system of partial differential equations results, where the shear velocity field is coupled nonlinearly to shear and normal stresses. This model reproduces theFerry model in various limits, but in general must be solved numerically. We use a numerical toolkit of one of the authors for reported simulations. We report threshold criteria in terms of the bulk imposed strain where nonlinearity leads to measurable experimental effects: in the shear wave or displacement field along the sample depth, and in shear and normal stress features. For various bulk strains (between 1 and 100%), we assess the errors in inverse characterization of storage and loss moduli due solely to nonlinearity, again specializing to conditions typical of ASLs.

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MS69

Effective Property Characterization of Nano-Composites From Homogenization and Percolation Theory

Many nano-composites consist of rod-like or platelet macromolecules in a solvent matrix, which are observed to yield large property enhancements at very low volume fraction. These particle suspensions are called liquid crystal polymers because they order at a critical volume fraction. In this talk, we study the role of the orientational distribution function of liquid crystal polymers and high aspect ratio particle dispersions in composite properties. We start with a review of the kinetic theory of owing rod dispersions. Then, we use homogenization theory to predict volume-averaged effective properties (specfically thermal conductivity and mechanical properties) versus particle volume fraction, aspect ratio and shear rate. The formulas we derive are in terms of second and fourth moments of the orientational distribution function of the inclusions. We close with recent progress on percolation in rod dispersions.

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MS70

Geometric Strategies for Neuroanatomic Analysis from MRI

Quantitative analysis of brain structure is important in the study of a variety of neurological and neuropsychiatric disorders. In addition, the accurate delineation of gray matter regions can provide important baseline information for quantifying brain function and metabolism. This talk will present a body of work grounded in the use of geometrical constraints and mathematical optimization to analyze neuroanatomical structure, function and metabolism of the human brain from Magnetic Resonance Images (MRI) and Magnetic Resonance Spectroscopic Imaging (MRSI). We will describe our applied mathematical approaches to the integrated analysis of cortical and subcortical the segmentation of cortical and subcortical structure, the analysis of white matter fiber tracks using diffusion tensor imaging (DTI) and the intersubject registration of neuroanatomical (aMRI) datasets. Many of our methods rally around the use of geometric constraints, statistical (MAP) estimation and the use of level set evolution strategies. In addition, more recently, we are combining the methods described here with functional MRI (fMRI) and MRSI analysis strategies with the goal of developing a more fully integrated approach to structural/functional/metabolic brain image analysis. We note that bringing all of this information into a common space via intra- and inter- subject registration should provide us with a rich set of data to investigate variation in the (normal, abnormal and developing) human brain.

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MS70
Diffeomorphic Metric Curve and Surface Matching

Curves and surfaces embedded in 3D are important geometric models for anatomical shape study in medical image analysis. A fundamental task in medical applications is to perform a non-rigid matching (deformation) between two occurrences of the same structure. Existing fully automated curve or surface matching approaches face two fundamental issues. One is that due to discretization, a point on one object need not have a homologous point on the other. The second issue is that geometric information is necessarily discarded when reducing curves or surfaces inherently 1D or 2D objects to 0-dimensional point sets. We develop curve and surface matching approaches in which the two issues mentioned above are overcome naturally in the fundamental theoretical framework by representing curve or surface geometry structure via currents. Our main contribution is in building a norm on the space of curves or surfaces via representation by currents of geometric measure theory. Currents are an appropriate choice for representations because they inherit natural transformation properties from differential forms. We impose a Hilbert space structure on currents, whose norm gives a convenient and practical way to define a matching functional. Using this Hilbert space norm, we also derive and implement curve and surface matching algorithms under the large deformation framework, guaranteeing that the optimal solution is a one-to-one regular map of the entire ambient space. We detail an implementation of curve and surface algorithms and present results on medical image data. Finally, one clinical application, cortical thickness variation of planum temporale in schizophrenia and bipolar diseases, is given using surface matching via currents.

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MS70
Quasiconformal Visuotopic Map Complexes in Human Brain: Methods and Motivations for Near-Isometric Brain Flattening

Brain imaging studies often require the representation and manipulation of highly convoluted cortical surfaces, generating three broad areas of application: visualization of surface data, metrically valid characterization of functional architecture in individual samples, and cross-subject comparison of anatomical or functional data. For visualization, any one-to-one, relatively undistorted representation is sufficient. However, for the latter two applications, careful attention to the metric aspects of surface mapping is critical. First, functional architecture studies are illustrated with the example of quasiconformal map complexes. These are physiological representations of the surface of the retina, relayed to the cortex in the form of multiple copies, or "maps" with shared boundary conditions, of a strongly non-linear, spatially warped retinal visual pattern. It has recently been demonstrated that composition of a complex dipole map (i.e. $w = \log(z + a/z + b)$) with a constant azimuthal shear map, indicates the existence of, and quantitatively describes, cortical "map complexes." These share the same conformal structure, but differ quantitatively in their anisotropy, or shear. Examples of wide-field (up to 70 degree) human visuotopic mappings, obtained with a newly developed optical system for fMRI based visual stimulation, will be shown. Secondly, ultra-high resolution (200 micron isotropic voxel) post-mortem human brain images, achieved via high field (7 Tesla) long duration (12 hour) MRI scans, are demonstrated. The goal is to measure the variance in "shape" of primary visual cortex, both within individual humans, and across monkey and human, as an example of cross-subject population comparison. Both applications require the development of maximally accurate, near-isometric flattening methods. Our current methods for brain flattening, based on the computation of exact minimal geodesic paths on polyhedral surfaces, together with metric multi-dimensional scaling, will be outlined. Metric distortion in the range of 5-10% is achievable by full distance matrix flattening, with computation times (16 Gbyte 3Ghz Opteron) of roughly ten hours for (10k polygon) cortical surfaces spanning V1,V2 and V3, i.e. most of the occipital pole. Although computationally expensive in time and memory, accurate metric representation of the brain surface is critical to the demonstration, presented here, that macaque and human map complexes have virtually identical visuotopic structure and and anatomical shape (V1), and that cross-subject population comparisons can be performed with high accuracy for areas such as primary visual cortex, especially in comparison with other current methods of population comparison of brain structure. Supported by NIH/NIBIB EB1550.

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MS70
Brain Surface Parameterization with Riemann Sur-

face Structure

We develop general approaches that parameterize brain anatomical surfaces with Riemann surface structure. All metric orientable surfaces are Riemann surfaces and admit conformal structure. With harmonic energy minimization, holomorphic 1-form and the Ricci flow methods, we can parameterize brain surfaces with various canonical surfaces such as sphere, Euclidean plane and punched hole disks. The resulting surface subdivision and the parameterizations of the components are intrinsic and stable. Our parameterization scheme offers a way to explicitly match landmark curves in anatomical surfaces such as the cortex, providing a surface-based framework to compare anatomy statistically and to generate grids on surfaces for PDE-based signal processing. Various applications of our research will also be discussed.

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MS71
Computational Methods for Leakage Estimation

One of the most likely pathways for leakage of injected CO2 is abandoned wells, especially in North America, where millions of wells have been drilled over the past century. The large disparity in length scales between overall CO2 plume size and localized leakage along wells, and the high uncertainty about materials within old wells, make the problem of leakage estimation very challenging. In this presentation, a range of computational methods will be explored to estimate CO2 leakage.

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MS71
Challenges in Modeling and Simulation of Geological CO2 Sequestration Processes

Geological sequestration of CO2 in depleted oil or gas reservoirs, deep aquifers or coalbeds is increasingly looked at as a viable way to reduce the atmospheric concentration of this greenhouse gas. To address the important questions of the feasibility, risks and costs of geological CO2 sequestration processes, researchers frequently turn to computer simulations. Reliable simulation is however extremely challenging. We discuss the current state-of-knowledge in geological CO2 sequestration, the numerical challenges, and the research required to advance this field.

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MS71
Numerical Modeling of CO2 Sequestration in Geological Formations

We present a model concept that is capable of describing the flow and transport processes of CO2 sequestration in aquifer systems due to advection and diffusion in the reservoirs. We further consider the mutual solubilities of CO2 and water/brine as well as the influence of phase composition on the fluid properties in the CO2-water system. The influence of heterogeneities and structures such as cap rock and wells and their implementation in the model with sophisticated preprocessing tools is discussed.

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MS71
Semi-Analytical Methods for Leakage Estimation and Risk Assessment

Estimation of the flow and migration of CO2 during the injection phases of a CO2 storage operation is greatly complicated by the presence of large numbers of abandoned wells. These wells act as potential conduits for leakage. This presentation covers the development of fast semi-analytical solutions to CO2 migration in systems of several aquifers connected by abandoned wells, and uses this semi-analytical framework to analyse a sample injection operation from a risk assessment perspective.

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MS72

Effects of Hydrodynamic Slip on Electrokinetic Phenomena

Abstract not available at time of publication.

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MS72

Induced-Charge Electro-Osmosis at Highly Charged Surfaces

t is well known that the classical Poisson-Nernst-Planck equations of electrokinetics predict nonsense for zeta potentials only a few times the thermal voltage (¿ 0.1 Volt), namely ion densities exceeding the physical limit, especially for large or multivalent ions at high ionic strength. In the traditional context of colloids, such large zeta potentials are uncommon (at least, near equilibrium), but in electromicrofluidics it is common to apply a volt or more across the double layer, to increase the flow rate. Even at lower operating voltages, it is clear that the standard model of a dilute solution must break down near the surface. A telltale sign is the as-yet unexplained, universal decay of nonlinear (induced-charge) electro-osmotic flow with increasing concentration (¿ 10 mM). Here, we propose a mathematical model of electrokinetics at highly charged surfaces which takes into account (i) steric effects of finite ion size and (ii) a concentration-dependent viscoelectric effect. We derive slip formulae for electro-osmosis and diffusioosmosis, which correct the classical theories of Smoluchoski and Deryagin, respectively, for flow saturation at highly charged surfaces. The theory predicts some interesting new phenomena, such as the induced-charge electrokinetic motion of an uncharged, ideally polarizable metal sphere in a uniform electric field, when the electrolyte is asymmetric.

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MS72

Going Beyond Mean-Field Theory: Electrolytes At Equilibrium Near Planar and Cylindrical Macromolecules

Equilbrium statistical mechanics of electrolytes is described, on the mean-field level, by Poisson-Boltzmann theory. I will discuss recent theoretical approaches that go beyond this approximation near charged macromolecules, having planar and cylindrical geometry.

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MS72

DNA Deformation in Complex Electric Fields

The ability to controllably position and stretch large DNA molecules in a microfluidic format is important for gene mapping technologies such as Direct Linear Analysis (DLA). Current technologies developed for DLA use controlled hydrodynamic flows created in a microfluidic device. The downside to this approach is that the imposition of the no-slip condition at the channel walls generates vorticity which can lead to DNA chain tumbling and incomplete stretching. We have recently shown that electric field gradients can be readily generated in a microfluidic device and the resulting field is purely elongational. We present here single molecule studies of DNA molecules driven by an electric field through a microfabricated contraction. Analogous to the hydrodynamic deformation of DNA, we can define an electrophoretic Deborah number (De) for our problem. We will discuss the effectiveness of the device to fully stretch DNA as a function of De and compare to stretching achieved in hydrodynamic flows. A detailed analysis of molecular stretching and the role of a non-homogeneous electric field will be discussed.

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MS73

Flow and Deformation in Swelling Porous Materials

Bio-tissue, highly-interacting soils such as clay, and swelling polymers such as what is used for drug delivery systems are all examples of swelling porous materials for which the coupling of flow and deformation may be of interest. The fundamental equations for flow and deformation in non-swelling porous materials include Darcy's law, which governs the rate at which fluid flows as a function of pressure gradient, and the Terzaghi stress principle, which governs the way in which an external load is distributed between the liquid and solid phases. Here we examine the assumptions of these traditional equations and develop a themodynamically admissible generalization of these two equations.

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MS73

Numerical Modeling of Complex Geometries and Processes in Hydrocarbon Reservoirs by the Dis-

continuous Galerkin and Mixed Methods

We present a numerical model for simulating water injection in fractured and faulted media in 2D and 3D. We combine the mixed finite-element (MFE) and discontinuous-Galerkin (DG) methods such that the former is used to solve the pressure equation and the latter is used for the saturation equation. This combination allows unstructured grids, low numerical dispersion, and natural modeling of complex fracture geometries. Results show the robustness and efficiency of our model in fractured media.

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MS73

Modeling Leakage of Carbon Dioxide from Underground Storage Sites

Reduction of atmospheric greenhouse gas is of great current interest. One mechanism for reducing carbon dioxide emissions is to capture and reinject these gasses into abandoned reservoirs. Regulators must then be able to determine whether these buried gasses will leak back out into the atmosphere or into underground “assets” such as active hydrocarbon reservoirs or aquifers with usable drinking water. We will discuss a simple modeling study to begin to answer questions of CO2 leakage.

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MS73

Pore-Scale Simulations of Reactive Transport with Smoothed Particle Hydrodynamics

A new Lagrangian particle model based on smoothed particle hydrodynamics (SPH) was used to simulate pore scale precipitation reactions. The Lagrangian particle nature of SPH allows physical and chemical effects to be modeled with relatively little code-development effort. In addition, geometrically complex and/or dynamic boundaries and interfaces can be handled without undue difficulty. The side-by-side injection of reacting solutions into two halves of a two-dimensional granular porous medium was simulated. Precipitation on grain surfaces occurred along a narrow zone in the middle of the domain, where the reacting solutes mixed to generate a supersaturated reaction product. The width of this zone was found to be practically independent of the Peclet number (Pe), but the precipitation rate increased with increasing Pe. The mixing zone decreased with time as precipitated minerals reduced contact between solutes A and B. The numerical simulations qualitatively reproduced the behavior observed in laboratory experiments.

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MS74

Gibbs Phenomenon and the Runge Phenomenon: New Strategies to Defeat Old Adversaries

Shock waves in plasmas and fronts in the ocean and atmosphere inflict Gibbs Phenomenon on spectral series. Gottlieb and others have developed a partial remedy: reprojection using Gegenbauer polynomials. We have shown that the Gegenbauer method sometimes diverges because of a generalized Runge phenomenon. Using a mix of numerical experiments and theory, we describe the strengths and weaknesses of alternatives including overdetermined polynomial fits and rational Chebyshev reprojection.

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MS74

High Order Limiting for Discontinuous Galerkin Methods

Discontinous Galerkin methods have been successfully used for numerical simulation of solutions of PDEs. When approximating the solution to hyperbolic PDEs with discontinuous solutions, we need some variety of limiting to reduce spurious oscillations near the discontinuity. In this talk, we present several modifications to limiting, including local and high order limiting.

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MS74

Aliasing Errors Due To Quadratic Non-Linearities

On Triangular Spectral/HP Element Discretisations

In this talk we present a study of how aliasing errors, introduced when evaluating non-linear products inexactly, affect the solution of Galerkin spectral/hp element polynomial discretisations on triangles. We present a theoretical discussion of aliasing errors introduced by a collocation projection onto a set of quadrature points insufficient for exact integration as well as considering interpolation projections to geometrically symmetric collocation points. The discussion is also corroborated with numerical examples which elucidate the key features of our arguments. We motivate our study with a review of aliasing errors introduced in one-dimensional spectral element methods (results which extend naturally to tensor-product quadrilaterals and hexahedra). For triangles, we show that integral quadrature rules developed on a non-rotationally symmetric, collapsed coordinate system minimize the magnitude of aliasing error introduced when insufficient quadrature order is adopted. If the Gaussian quadrature order employed is less than half the polynomial order of the integrand, then it is possible for the aliasing error to modify the constant mode of the expansion and therefore affect the conservation property of the approximation. However the use of a collocation projection onto a polynomial expansion associated with a set of rotationally symmetric nodal points within the triangle are always observed to be non-conservative. Nevertheless the rotationally symmetric collocation will maintain the overall symmetry of the triangular region which is not typically the case when a collapsed coordinate quadrature projection is used.

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MS74

A Hybrid Fourier-Chebyshev Pseudo-Spectral Method for Non-Periodic Hyperbolic Problems

Fourier pseudo-spectral methods produce outstanding results for smooth problems with periodic boundary conditions. For non-periodic problems, Chebyshev pseudo-spectral methods are commonly used to obtain exponential rates of convergence. However, while Fourier methods require 2 points per wavelength, Chebyshev methods require π. Moreover, the clustering of nodes near the boundaries required by polynomial methods also impose an $O(1/N^2)$ restriction on the time-step size when these methods are used for hyperbolic problems. In order to circumvent these difficulties in the solution of non-periodic problems, we propose a hybrid Fourier-Chebyshev pseudo-spectral method. The method requires a cut-off function w, where w and its derivatives are approximately zero at the boundary. The target function u is then replaced by the product uw which is periodic and can be accurately approximated by a trigonometric series. A polynomial approximation is needed only in the region where w is close to zero (near the boundaries), since u cannot be accurately recovered from uw if w is small. Numerical results confirm the spectral accuracy and stability of the method. Because w may have large gradients, the method is particularly suitable for stiff problems.

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MS75

Review of Finite-Difference Gaussian Rules

Finite-difference Gaussian rules or optimal grids were introduced for accurate computation of Dirichlet-to-Neuman maps using second order finite-difference schemes in late 90s. Since then they have shown great success in many applications in oil industry. I review some basic theory of the optimal grids and their applications to electromagnetic and acoustic well logging and also to oil reservoir optimization developed at Schlumberger.

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MS75

A Simple Finite-Element Alternative to Optimal Finite-Difference Grids

Optimal grids, which are largely limited to FDM, are not accessible to a large community that uses standard Bubnov Galerkin FEM. This talk outlines a highly accurate FEM that is similar to the optimal grid FDM. By linking special-quadrature FEM to rational approximations, we develop an extremely simple yet powerful discretization technique applicable to a broad class of problems where the governing differential equation is second-order in space (e.g. elastostatics, wave propagation and subsurface imaging).

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MS75

Optimal Grids for the Electric Impedance Tomography problem

We present a numerical inversion method for a one-dimensional inverse spectral problem related to Electrical Impedance Tomography, where the conductivity is sought from spectral data. First we find the sparsest resistor network reproducing the available spectral data, then the resistors are interpreted as averages of the conductivity over a precomputed grid, that is optimal for a reference conductivity. A Gauss-Newton procedure is used to improve the reconstructions when a priori information about the solution is available.

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MS75
Solution of Multidomain Anisotropic Problems

Optimal grids yield spectral convergence of the Neumann to Dirichlet map for an isotropic problem on a square, and this is the reason that they work so well for multi-domain isotropic problems. We extend this technique to multi-domain anisotropic problems for applications to borehole models with deviated wells. The anisotropy corresponds to a shift in the domain of the spectral approximation from the real axis to a ray in the complex plane.

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MS76
Fast Algorithms for Polynomial Vandermonde Matrices Related to Quasiseparable Matrices

While general matrix algorithms are known to require $O(n^3)$ operations, the special structure of Vandermonde and Vandermonde-related matrices allows computational savings resulting in algorithms of only $O(n^2)$ operations for certain special classes. Specific classes that have already been considered are classical Vandermonde matrices, Chebyshev-Vandermonde matrices, three-term Vandermonde matrices, and Szegö-Vandermonde matrices. In each the known algorithms for inversion and for solving a linear system are of the lower $O(n^2)$ complexity. In this paper we consider the most general special class of quasiseparable-Hessenberg-Vandermone matrices that generalize all the above classes. We derive generalizations of the well-know Bjorck-Pereyra and Traub algorithms. The results of numerical experiments will be presented.

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MS76
On a Class of Shifted Quasiseparable Matrices

We consider a class of structured matrices with a rank structure below some subdiagonal and above some superdiagonal. This is a generalization of a class of quasiseparable matrices we studied previuosly. We study the basic properties of this class of matrices. Using the rank structure we derive for such matrices fast inversion, QR factorization and eigenvalue computation algorithms.

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MS76
Eigenvalue Problems for Quasiseparable Structures

Recently the exploitation of quasiseparable structures in the context of the matrix eigenvalue problem has lead to a significant computational breakthrough. In this talk we summarize our results, present some fast eigenvalue algorithms and discuss numerical issues which are to be addressed in their implementation.

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MS76
A Movie of Elimination

Direct elimination on a sparse matrix produces fill-in that depends on the ordering of the rows. The fill-in appears in the LU factors, and this determines the cost of elimination (and the storage required). We consider matrices whose nonzero structure is given by a graph, so different row and column orderings correspond to orderings of the nodes. We illustrate the elimination process by a movie. The graph shows the degree of each node (changing as elimination proceeds). The nonzeros in the matrices and the floating-point operations are counted. For the 5-point Laplacian we include the natural order (poor) and nested dissection, and the approximate minimum degree algorithms developed by Tim Davis.

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MS77
Do We Owe HIV Resistance to Smallpox?

The high frequency, recent origin and geographic distribution of the CCR5-Δ32 deletion allele together indicate that the allele has been intensely selected in Europe. While the allele confers resistance against HIV-1, HIV has not existed in the human population for long enough to account for this selective pressure. The prevailing hypothesis is that the selective rise of CCR5-Δ32 to its current frequency can be attributed to bubonic plague. Results from a population genetic framework that takes into account the temporal pattern and age-dependent nature of specific diseases indicates that smallpox is more consistent with this historical role. Future research possibilities for models that integrate population genetics with epidemiological dynamics will be discussed.

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MS77

Vector Borne Diseases with Structured Vector Populations: Extinction and Spatial Spread

We derive from a structured population model a system of delay differential equations describing the interaction of five sub-populations, namely susceptible and infected adult and juvenile host and infected adult vector, for a vector-born disease with particular reference to West Nile virus, and we also incorporate the spatial movements by considering the analogue reaction-diffusion systems with non-local delayed terms. Specific conditions for the disease eradication and sharp conditions for the local stability of the disease free equilibrium are obtained using comparison techniques coupled with the spectral theory of monotone linear semiflows. A formal calculation of the minimal wave speed for the traveling waves is given and compared with filed observed data.

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MS77

Statistical Modeling of Influenza as a Diffusion Process

Medical geographers have studied the transmission of influenza at the population level as a diffusion process for decades. Mathematical models that incorporate diffusive effects have been developed in tandem. Despite work in these related areas, statistical modeling has generally lagged in developing true spatio-temporal models for influenza transmission across large temporal and geographic scales. Careful quantification of spatio-temporal dynamic parameters for the disease process can be further strengthened and extended. We will introduce some basic methods and models to investigate diffusion of influenza from a statistical modeling perspective, and apply these methods to 40 years of influenza surveillance data from the United States.

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MS77

New Insights into Hepatitis B Virus Infection Dynamics

About 300 million people worldwide are infected with hepatitis B virus. Upon infection about 85% of adults clear the virus while the remaining 15% go on to develop chronic disease. I will introduce a new class of mathematical models that describe acute hepatitis B virus infection that attempt to address the roles of antibody as well as cytolytic and noncytolytic immune responses in clearing HBV infcetion.

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MS78

Studies of the Nonlinear Evolution of the m=1 Sawtooth Mode in Extended MHD Models Using Adaptive Mesh Refinement

Reconnection observed in nature is often impulsive, which resistive MHD cannot explain. However extended (including two-fluid effects) MHD models indeed show accelerated growth nonlinearly. We present simulations of the m=1 tearing mode (important e.g. for sawtooth oscillations in tokamaks), in reduced 2d as well as fully 3d extended MHD models. Our code employs block-structured quad-/octtree based adaptive mesh refinement, load-balanced via Hilbert-Peano curves. The arising elliptical equations are solved using a fast adaptive multi-level method.

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MS78

Fully Implicit Adaptive Mesh Refinement for Reduced Resistive Magnetohydrodynamics

Application of implicit adaptive mesh refinement (AMR) to simulate resistive magnetohydrodynamics is described. Solving this challenging multi-scale, multi-physics problem can improve understanding of reconnection in magnetically-confined plasmas. Implicit time integration is used to step over fast Alfven time scales. At each time step, large-scale systems of nonlinear equations are solved using Jacobian-free Newton-Krylov methods together with a physics-based preconditioner on AMR grids. LAUR's 04-7312,04-9024,05-2645

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MS78

Adaptive Mesh Simulations of Pellet Injection in Tokamaks

We present results of 3D extended MHD AMR simulations of pellet injections into tokamaks which span several

decades of space-time scales. The large disparity between pellet and device size, large density differences between the pellet ablation cloud and ambient plasma, and the non-local electron heat transport all pose numerical challenges. Block structured AMR, using Chombo, extended to equilibrium magnetic coordinates, is employed to deal with the large range of spatial scales. Supported by USDOE Contract no. DE-AC020-76-CH03073.

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MS78

Block-Adaptive Parallel Explicit/implicit MHD Simulations in Space Physics: the Art of Compromise

Space physics simulations require the resolution of disparate spatial and temporal scales. Space weather prediction further requires that the 3 dimensional time accurate problem be solved faster than real time. To achieve an efficient and accurate spatial discretization we employ a block adaptive grid that is well suited for massively parallel supercomputers. To overcome the time step limitations of the explicit time stepping, we have developed a parallel explicit/implicit time integration scheme on the block-adaptive grid. The basic idea of the algorithm is that the time stepping scheme can differ in the blocks of the grid for a given time step: an explicit scheme is used in the blocks where the local stability requirement is not violated and an implicit scheme is used in the blocks where the explicit scheme would be unstable. The implicit scheme is second order in time. The non-linear system of equations is linearized with Newton linearization. The linear system is solved with a preconditioned Krylov subspace iterative scheme. The Schwarz type preconditioning is also based on the block structure of the grid. We discuss the optimal choice of parameters for the Newton-Krylov-Schwarz scheme, the load balancing for parallel execution, and the optimal choice of the time step for speed and robustness. The control of the numerical divergence of the magnetic field in combination with the explicit/implicit time stepping scheme is also discussed. The accuracy, robustness and parallel efficiency of the algorithm are demonstrated on test problems as well as for three dimensional time dependent space physics applications.

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MS79

New Formulae for Conformal Mapping to Multiply Connected Polycircular-Arc Regions

A polycircular arc region is a generalization of a polygonal region and is a planar domain whose boundaries consist entirely of circular arcs. An analytical framework for constructing conformal mappings to simply connected polycircular arc regions is well-known. In this talk, we present new formulae for the construction of conformal mappings to multiply connected polycircular arc regions.

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MS79

Multiply Connected Schwarz-Christoffel Mapping: Some Theoretical Aspects

We will give an overview of Schwarz-Christoffel transformations for conformal maps from multiply connected domains bounded by circles to domains bounded by polygons. The derivation of the formulas using a reflection argument will be presented and the relation of our formulas to a similar formula due to D. Crowdy will be discussed. Other theoretical aspects, such as the convergence of the resulting infinite product representation for the derivative of the map, will also be outlined.

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MS79

Developing a Computational Framework for Conformal Mapping

There are now many mature computational methods and several publicly available packages for conformal mapping. Since conformal maps are a means rather than an end, software needs to be put into a context that allows users to implement common applications quickly and develop customized ones if desired. I will describe an object-based MATLAB environment that will allow users to work with piecewise analytic, multiply connected, and unbounded geometries, and conformal maps to them.

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MS79

Some Applications of Schwarz-Christoffel Transformations in Higher Connectivity

For a multiply connected domain the complex plane there are several possibilities for a canonical domain for conformal images. We will consider circular domains and parallel slit domains. The recently derived Schwarz-Christoffel formula for mappings to a polygonally bounded, multiply connected domain from a circular domain will be used to give a variety of applications. These include fluid flows and inverse problems. For example for a bounded domain the canonical circular domain can be taken to be the unit circle with smaller disks removed and two such maps yield the map to a rectangle with parallel slits. This yields immediately the resistance of a quadralateral obtained from four marked points on the outer boundary of the polygonal domain. For the determination of several cracks in the polygonal domain a generalized Schwarz-Christoffel parameter problem can be formulated as has been done previously for singly and doubly connected domains by the author and co workers.

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MS80

Progress and Problems in Electrical Impedance Tomography

Electrical Impedance Imaging systems apply currents to and measure the resulting voltages on the surface of a body. From this electrical data images are reconstructed and displayed of the electrical conductivity and permittivity inside the body. Mathematically the reconstruction of these functions is an inverse boundary value problem for Maxwell's equations. Since hearts filled with blood , lungs filled with air , and breast tumors all have significantly different conductivities from hearts depleated of blood, lungs depleated of air , and normal breast tissue respectively these images can be used to monitor heart and lung function and to diagnose breast cancer. Mathematical problems that arise in designing Adaptive Current Tomography (ACT) systems will be described . Images and movies of heart and lung function as well as preliminary images of breast cancer made by the ACT3 and 4 systems will be presented.

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MS80

Kronecker Product Approximation for Preconditioning in 3D Imaging Applications

We derive Kronecker product approximations, via tensor decompositions, to severely ill-conditioned matrices that arise in three-dimensional image processing applications. We use our approximations to derive preconditioners for iterative regularization techniques; the resulting preconditioned algorithms allow us to restore three dimensional images in a computationally efficient manner. Through examples in microscopy and medical imaging, we show that the Kronecker approximation preconditioners provide a powerful tool that can be used to improve efficiency of iterative image restoration algorithms.

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MS80

Image Reconstruction Algorithms for Optical Tomography with Large Data Sets

There has been considerable recent interest in the image reconstruction problem in optical tomography with diffuse light. In this talk we review recent progress on the development of fast image reconstruction algorithms. The algorithms derive from the analysis of the inverse scattering problem for the radiative transfer equation and are suitable for use with data sets as large as 10^{10} measurements. Numerical simulations and experimental data from model systems are used to illustrate the results.

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MS80

Optical Tomography with Large Data Sets

This talk will discuss the development of fast algorithms for the image reconstruction problem in optical tomography. The algorithms are tested on experimentally derived data sets with 10^8 source-detector pairs.

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MS81

A Stoichiometric Constraints-Based Approach to Modeling Melanoma Cells

It is thought that melanoma cells may be able to evade normal cell growth controls because of specific changes in the expressed genes and splice variants of metabolic proteins and growth regulatory proteins. The tumor cells may also be predisposed to handle hypoxic conditions due to changes in glucose and fatty acid metabolism. To test these claims, I will present results from a stoichiometric constraints-based optimization approach.

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MS81

Evaluating the Benefits of Colorectal Cancer Screening

Although there is solid evidence of the efficacy of colorectal cancer screening, the optimal screening strategy is a topic of constant debate. Using multistage carcinogenesis models, we construct mathematical expressions for the number and size distribution of premalignant lesions in the colon and the rectum (aberrant crypt foci and polyps) at any particular age. We use such expressions to evaluate the effects of different screening and intervention strategies in colorectal cancer risk.

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MS81

Gestational Mutations and the Risk of Cancer

During this talk we present a mathematical formulation designed to evaluate the effects of gestational mutations on cancer risk. Models for the accumulation of critical mutations during gestation (Luria-Delbruck type) are used in tandem with multistage models of carcinogenesis to derive hazard and survival functions of cancer in specific tissues. To illustrate the uses of the methodology, we present estimations of the proportion of colorectal cancers in the US population that could be attributed to gestational mutations, and discuss the consequences of in utero X-Ray exposures on cancer risk. We conclude this talk with a discussion of the necessity to account for gestational mutations in order to explain the characteristic age-specific incidence of Acute Lymphoblastic Leukemia (ALL) in children.

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MS81

T Cell Recirculation and HIV Infection

Standard models of HIV dynamics within humans treat the body as a homogeneous medium with free mixing of virus and T cells. However, experimental and clinical work has revealed that HIV preferentially depletes CD4 T cells associated with mucosal tissues. In this talk, I'll present a compartmental model of *in vivo* T cell dynamics and HIV's effect on those dynamics. The predictions will be compared to experimental results, and the implications for HIV treatment are discussed.

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MS82

Large-Scale Inverse Transport: Multigrid Methods and Uncertainty Quantification

We are interested in the localization of airborne contaminant releases in regional atmospheric transport models from sparse observations, in time scales short enough for predictions to be useful for hazard assessment, mitigation, and evacuation procedures. In particular, our goal is rapid reconstruction—via solution of an inverse problem—of the unknown initial concentration of the airborne contaminant in a scalar convection-diffusion transport model, from limited-time spatially-discrete measurements of the contaminant concentration, and from a velocity field as predicted, for example, by a mesoscopic weather model. We discuss special-purpose multigrid methods for rapid solution of the inverse problem, as well as techniques to estimate and propagate the resulting uncertainty in the intial condition field.

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MS82

Multilevel Algorithms For Large-Scale Interior Point Methods In Bound Constrained Optimization

We develop and compare multilevel algorithms for solving bound constrained nonlinear variational problems via interior point methods. Several equivalent formulations of the linear systems arising at each iteration of the interior point method are compared from the point of view of conditioning and iterative solution. Furthermore, we show how a multilevel continuation strategy can be used to obtain good initial guesses ("hot starts") for each nonlinear iteration. A minimal surface problem is used to illustrate the various approaches.

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MS82

Feasible and Non-Interior Path-Following in Con-

strained Minimization with Low Multiplier Regularity

Primal-dual path-following methods for constrained minimization problems in function space with low multiplier regularity are introduced and analyzed. Regularity properties of the path are proved. The path structure allows to defined approximating models which are used for controlling the path parameter in an iterative process for computing a solution of the original problem. The Moreau-Yosida regularized subproblems of the new path-following technique are solved efficiently by semismooth Newton methods. The overall algorithmic concept is provided and numerical tests (including a comparison with primal-dual path-following interior point methods) for state constrained optimal control problems show the efficiency of the new concept.

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MS82
Assessing the Performance of Optimization-Based Multigrid Methods

Many large nonlinear optimization problems are based upon discretizations of underlying continuous functions. Optimization-based multigrid methods are designed to solve such discretized problems efficiently by taking explicit advantage of the family of discretizations. The methods are generalizations of more traditional multigrid methods for solving partial differential equations. We discuss techniques whereby the multigrid method can assess its own performance, with the goal of adaptively deciding appropriate levels of discretization.

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MS83
Gauss-Arnoldi Quadrature for $\langle (zI - A)^{-1}\phi, \phi\rangle$ and Padé-Like Approximation of Markov Type Functions

Quality of Gauss–Arnoldi quadrature for computation of $\langle (zI - A)^{-1}\phi, \phi\rangle$ is studied, where A is a bounded operator in Hilbert space and φ is a nonzero vector. We have established optimistic and pessimistic results on the quadrature's effectiveness. Relation to PTA (with poles at Ritz numbers) enables us to localize the poles of "rational perturbations". The obtained error estimates are applicable even when the classical Padé approximation doesn't work. The results of numerical experiments are presented.

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MS83
Optimal Discretization of PML for Elasticity Problems

We present an original approach of Perfectly Matched Layers construction. This approach is based on the Optimal Gerids techniques. This PML allows one to reach suitable reduction of the reflections for all the incident angles. The approach makes it possible totally decrease the computational time because high precision of the solution can be reached using small number of grid points.

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MS83
Optimal Grid-Based Methods for Thin Film Micromagnetics Simulations

Pseudodifferential operators, such as the Dirichlet-to-Neumann map for the Laplace's equation in half-space often arise in nonlinear problems, and, in particular, in the context of pattern formation. Efficient numerical methods can therefore be very useful in understanding the spatiotemporal dynamics in these complex nonlinear systems. In this talk, I will discuss several implementations of optimal grids for the numerical studies of the domain wall structures in thin film micromagnetics and present an important new type of solutions found in these studies.

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MS83
Finite-Difference Solution of the 3D Electromagnetic Problem Using Optimal Grids

We solve 3D fully anisotropic Maxwell's equation in unbounded domains for electrical prospecting. We use optimal grids for approximation in the exterior part of infinite domain. Special averaging procedure is used to account for inhomogenuity.

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MS84

A Polymeric Assembly and Disassembly Model for Min Oscillations

In this paper, we study a mathematical model for MinCDE oscillations which shows that diffusion and membrane binding can account for the pattern of spatial and temporal variation of the Min system. The model treats directed assembly of membrane-associated polymeric structures, and results in repeated cycles characterized by the following sequential events: 1. assembly of the MinD polar zone, beginning at a cell pole and growing to midcell; 2. assembly of the MinE ring at the medial edge of the polar zone; 3. vectorial disassembly of the polar zone from midcell to the pole while maintaining the association of the E-ring with its medial edge; 4. repetition of the same process at the other pole. The model also assumes reasonable associations of the Min molecules with each other and with membrane, consistent with known biochemical data. In addition, the model suggests that the physical structure of the membrane assembly is not crucial to the oscillations. Specifically, there is no difference between a system where the membrane structure is uniformly distributed around the periphery and a system where the membrane association occurs along a membrane-associated structure, such as a cytoskeletal element. We also discuss the role of nucleation sites for the attachment of the polymeric structure to the membrane.

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MS84

Stochastic Models for Dynamic Subcellular Protein Patterning

We discuss mathematical models of two systems involving intricate subcellular protein dynamics: the MinCDE system regulating accurate cell division in E. coli and the Spo0J/Soj system involved in chromosome segregation and transcriptional regulation in B. subtilis. We introduce fully stochastic models for each and discuss the importance of stochasticity when modelling spatiotemporal protein dynamics. We also examine the partitioning of the Min/Spo0J/Soj proteins at cell division between the two daughter cells. Current models predict that the copy numbers are not equalized between the daughter cells and hence that additional mechanisms are needed to preserve appropriate concentration levels.

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MS84

The Beginning of the Ends: a Molecular Study of the Origin of Min Protein Oscillations

The remarkable accuracy of cell division in E. coli and related bacteria is partially regulated by the Min-protein system, which prevents division near the cell ends by oscillating spatially from pole to pole. We have developed a model of the Min system, using only known properties of the proteins, which accurately reproduces the observed oscillations and predicts a finite nucleotide exchange rate for the MinD protein of around one second. In addition, we have extended our model to round cells to show that Min oscillations can spontaneously select the long axis of the cell to define the division plane in cocci. Our recent work focuses on particle-level simulations in rod-shaped cells, to study the impact of polymer formation by the Min proteins. These particle-level simulations provide a starting point to understand how prokaryotes and eukaryotes can use protein reaction-diffusion systems to detect their own geometry and target proteins to different locations in the cell.

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MS84

Simulating the Min System in *Escherichia coli*: Two Models of Oscillating Polymer Chains

The method by which *Escherichia coli* reproduces is to divide at its midplane to produce two roughly equal daughter cells. Failure to divide equally results the death of the cell line. Cell division in *E. coli* is regulated by the MinCDE system, composed of three proteins that work in tandem with each other to “measure” where the middle of the cell is. Polymer chains composed of the MinD protein assemble on the membrane and grow out from the polar ends of the cell towards the middle of the cell. The MinE protein attaches to the growing end of the polymer chain and then disassembles the chain. The newly released MinD and MinE diffuse through the cytoplasm, and a new set of chains assembles in the other pole. Two mathematical models of the MinCDE system will be presented. The first is a Markov model governed by a system of differential equations that describe the probability of finding a polymer chain with i MinD and j MinE proteins at time t. The second model is a Monte Carlo simulation that builds the polymer chains molecule by molecule. Unique to these two models is the use of neighboring interactions, where the state of one polymer chain can influence the rate at which its neighbors change. In the Markov model, these neighboring interactions are in the form of nonlinear polynomial transition rates, while in the Monte Carlo model, the neighboring interactions are implemented explicitly. Each of the models is simulated numerically. Multiple Monte Carlo simulations make it possible to determine the coefficients of the nonlinear rates in the Markov model. The Monte Carlo simulations showed clear oscillations; these oscillations support the biological theory that the polymer chains must form a bundle with neighboring interactions for oscillations to occur. However, even after the implementation of the coefficients from the Monte Carlo model, the Markov model did not oscillate. Oscillations will likely never be seen in this model as it simulates the average *E. coli* cell; thus, the Markov model smears out the oscillations seen in the individual Monte Carlo simulations.

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MS85

Stong Stability Preserving SDIRK Methods

Much attention has been paid in the literature to strong stability preserving (SSP) Runge-Kutta methods in the solution of ordinary differential equations (ODEs) coming from a semi-discrete, spatial discretization of time dependent partial differential equations (PDEs). Althoug in important situations it is natural to deal with implicit Runge-Kutta methods which are SSP, the attention has been essentially given only to explicit Runge-Kutta methods. In this talk we present singly diagonally implicit Runge-Kutta (SDIRK) methods which have the favourable property of being SSP. The conclusions that will be presented were obtained, at Leiden University, in a joint search with Marc Spijker.

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MS85

Positivity and Monotonicity for IMEX Methods

Space discretization of some time dependent partial differential equations (PDEs) give rise to ordinary differential equations (ODEs) containing additive terms with different stiffness properties. In these situations, with the aim to efficiently integrate the ODE with low computational cost, IMEX (IMplicit-EXplicit) Runge-Kutta methods are used. Furthermore, sometimes the solutions to these PDEs have qualitative properties (norm, energy, entropy, total variation diminishing, positivity, etc) that represent important physical features of the problem. In this case, in order to preserve the physical meaning of the numerical solutions, it is important to maintain these properties with both the spatial discretization and the time stepping method. Some IMEX Runge-Kutta can preserve positivity and monotonicity properties of the exact ODE solutions under certain stepsize restrictions. In this talk, we will show how it can be achieved.

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MS85

Variable Step-Size IMplicit-EXplicit Linear Multistep Methods

Implicit-explicit (IMEX) linear multistep schemes are popular methods for the time evolution of certain spatially discretized PDEs. These methods are designed to treat the stiff parts of the corresponding ODE systems implicitly and the nonstiff parts explicitly. IMEX multistep methods are defined for constant step-sizes. For solutions with different time scales, however, variable step-size schemes are often desired. In this talk we discuss some new second-, third- and fourth-order variable step-size IMEX multistep schemes. Numerical tests are also provided which illustrate the superiority of variable step-size IMEX schemes over classical schemes in a variety of situations.

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MS85

Comments on Linear Instability of Time Integration Methods with the Fifth-Order WENO Spatial Discretization

The weighted essentially non-oscillatory (WENO) method is a popular spatial discretization method for hyperbolic partial differential equations. We show that the combination of the fifth-order WENO spatial discretization (WENO5) and the forward Euler time integration method is linearly unstable when numerically integrating hyperbolic conservation laws. Moreover strong-stability-preserving (SSP) time integration methods offer no stability advantage over non-SSP methods when coupled with WENO5. We give new linear stability criteria for combinations of WENO5 with general ERK methods of up to order four. We confirm our analysis by means of numerical tests.

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MS86

New Preconditioning Techniques in Matrix Computations

We propose new preconditioning techniques for solving general and structured linear systems of equations and extend them to various other fundament al matrix computations such as computing rank, determinant, null vectors, eigenvalues and eigenvectors of a general or structured matrix. Our analysis and experiments show the efficiency of these techniques.

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MS86

Iterative Methods for Linear Systems with a Nearly Symmetric Matrix

Linear systems of equations with a matrix that the is sum of symmetric and low-rank matrices arise in various applications, e.g., from the discretization of certain boundary value problems for partial differential equations. This talk discusses iterative methods with short recurrence formulas for the solution of this kind of linear systems.

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MS86

Majorization and Toeplitz Tools in PDEs Preconditioning

We consider the FD discretization with minimal (centered) formu-
lae of precision 2 of the test convection-diffusion problem $A_{a,p}u \equiv -\nabla^T[a(x)\nabla u(x)] + \sum_{j=1}^{d} \frac{\partial}{\partial x_j}(p_j(x)u(x)) = g(x)$, $x \in \Omega$, with Dirichlet boundary conditions. Here Ω is a plurirectangle of $\mathbf{R}^d$, $a(x)$ is a uniformly positive function, and $p_j(x)$ denotes a bounded function on Ω for every $j = 1, \ldots, d$ (for plurirectangle we mean a connected union of rectangles in d dimensions with edges parallel to the axes). The idea is to use structured preconditioners for the matrices A_n arising from the FD approximation of the above problems: the spectral analysis of the corresponding preconditioned matrices is carried out by using tools from the Majorization Theory, especially the Weyl Majorant Theorem (see e.g. the beautiful book by Bhatia, Matrix Analysis, Springer, 1999) and from the spectral theory of Toeplitz sequences (see e.g. A. Böttcher, B. Silbermann, Introduction to Large Truncated Toeplitz Matrices, Springer, 1998 and for more recent results see Serra Capizzano, Generalized Locally Toeplitz sequences: spectral analysis and applications to discretized Partial Differential Equations, LAA 366-1 (2003), pp. 371–402).

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MS86

Development and Applications of Circulant-Plus-Low-Rank Approximation Techniques

Recent research has made it clear that good preconditioners should approximate the target matrices in some norm only up to a matrix whose rank is sufficiently small. This observation may serve as a base for new preconditioning techniques. If A is a given matrix and C is a preconditioner, then C is sought so that $A - C = R + E$, where the rank of R is as small as possible under the constraint $||E|| \leq \varepsilon$. This is an interesting and nontrivial approximation problem. We have discovered recently that this problem can be solved very efficiently if C is a circulant. The purpose of this talk is to develop and generalize our constructions to some other classes of structured matrices, including also multilevel matrices.

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MS87

Reliable Multiprecision Implementation of a Class of Special Functions

Special functions are pervasive in all fields of science and industry, in physics, engineering, chemistry, computer science and statistics. However, algorithms with strict bounds on truncation and rounding errors are not generally available for the evaluation of these functions. Since a lot of them enjoy very nice and rapidly converging limit-periodic continued fraction representations, we show how these representations are useful in a reliable multiprecision implementation. We guarantee a relative error bounded above by 1 ULP.

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MS87

Asymptotic Analysis of Higher-Order Derivatives of the Inverse Error Function

The inverse of the error function, inverf(x), has applications in non-linear heat theory, financial derivatives, turbulent combustion, and scalar field dynamics. It occurs in the solution of concentration-dependent diffusion and chemical potential problems. It is also used in computing confidence intervals in statistics and in some algorithms for generating Gaussian random numbers. We analyze $\mathrm{inverf}^{(n)}(0)$ asymptotically as $n \to \infty$, using Nested Derivatives and the Ray Method. We obtain a very good approximation of $\mathrm{inverf}(x)$ through a high-order Taylor expansion around $x = 0$. We give numerical results showing the accuracy of our formulas.

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MS87

Orthogonal Polynomials and Gaussian Quadrature Applied to the Solution of Large-Scale Ill-Posed Problems

The solution of large-scale ill-posed problems has recently received considerable attention. Many of the available solution methods are based on Tikhonov regularization. Part of the computational task is to determine a suitable value of the regularization parameter used in Tikhonov regularization. This talk describes iterative methods for Tikhonov regularization based on the Lanczos process and discusses how the regularization parameter and solution can be computed efficiently by using the connection between the Lanczos process, orthogonal polynomials, and Gaussian quadrature.

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MS87

Improved Calculation of Mathieu Functions of Integer Order with Application to Radiation from Pistons on An Elliptic Cylinder

Series expressions traditionally used to calculate the radial (i.,e., modified) Mathieu functions of integer order are shown to suffer significant subtraction error for many parameter choices. This includes the Bessel function product series which has an integer offset for the order of the Bessel functions that is traditionally chosen to be zero (or one). We have found that the use of larger offset values that tend to increase with increasing radial function order usually eliminates the subtraction error. A Fortran computer algorithm based on our results provides accurate values of radial Mathieu functions together with the associated angular functions over far wider parameter ranges than previously possible. We describe the application of the algorithm to the calculation of acoustic radiation from pistons on an elliptic cylinder.

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MS88

Application of Interior Penalty Galerkin Method to Inverse Problem

Optical tomography is a way to probe highly scattering media using low-energy visible light, and then reconstruct images of these media. It is well-known that the resulting diffusion optical tomography inverse problem is ill-posed. In this work, we investigate the effect of continuous finite element method versus nonsymmetric interior penalty Galerkin method for solving this ill-posed problem. We show that the continuous Galerkin inversion with L^2 smoothing term such as Tikhonov regularization differs from the discontinuous Galerkin solution with the same regularization. We also show that increasing the polynomial degree in the discontinuous Galerkin inversion, produces a more accurate solution.

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MS88

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS88

Modeling and Simulation of Electrodeposition in 2D and 3D

Judy and Motto have developed a modified electrodeposition process to fabricate very small metal structures on a substrate. Layers of metal of various shapes are placed on the substrate, then the substrate is placed in an electroplating solution. Some of the metal layers have power applied to them, while the rest of the metal layers are not connected to the power initially. Metal ions in the plating solution start plating the powered layers and a surface grows from the powered layers. As the surface grows, it may touch one of the metal layers that was not initially powered. This causes the initially unpowered metal layer to become powered, and it will start growing with the rest of the surface. The metal layers on the substrate are known as seed layer patterns, and different seed layer patterns can grow different shapes. In this paper, we model and simulate the growth of a surface from a seed layer pattern. A simple model of uniform growth in the direction normal to the surface is made, and the level set method is used to simulate the growth computationally in 2D and 3D. An inverse problem, which is to determine a seed layer pattern that would produce a given surface shape, is also addressed in 2D and 3D. Some given surface shapes may not be attainable by any seed layer pattern, and some conditions for attainable shapes are given.

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MS88

Mathematical Approaches for Global Ionospheric Data Assimilation

The Earth's ionosphere plays an important role in wireless communications between satellites ground receivers. Mathematical techniques of parameter estimation form the basis for the development of global ionospheric data assimilation models. Known in the ionospheric monitoring community as Global Assimilative Ionospheric Model, GAIM represents the most advanced ionospheric monitoring and forecasting tool available for civilian and defense applications.Our team of researchers at the University of Southern California and the Jet Propulsion Laboratory are among the first developers of GAIM. In this talk, the mathematical approached used in GAIM and the numerical implementation of GAIM are presented. The validation and operational performance of the model are also reported. Mathematical challenges for improving model accuracy for monitoring and forecast will be discussed.

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MS89

Sensitivity Analysis and Control for Systems Governed by Partial Differential Equations

This presentation summarizes results from efforts to combine continuous sensitivity equation methods with optimal control techniques in order to design controllers for systems governed by partial differential equations. The focus of the research is to use these ideas for the optimal placement of sensors and actuators for control designs related to Micro Air-Vehicle technology. In our approach sensor/actuator placement is parameterized, and the pde models are implicitly differentiated with respect to these parameters in order to obtain sensitivity information. Preliminary efforts show that this process can result in sensitivity information which is qualitatively believable but quantitatively questionable. A example using piezoceramic patch actuators on an Euler-Bernoulli beam illustrates some of the computational issues.

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MS89

Sensitivities in Eddy Viscosity Models

This presentation discusses the sensitivity of eddy viscosity models with respect to the variation of eddy viscosity parameter. We demonstrate the analysis utilizing the sensitivity equation method and provide numerical assessments to justify the application of our sensitivity computations.

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MS89

Mathematical Modeling of Cilia Sensors for Flow Control Applications

Autonomous micro air vehicle (MAV) flight faces inherent stability challenges. One challenge is controlling flow separation over the airfoil. An autonomous control system for MAV flight may be enhanced with closed loop separation control. In this talk, we focus on modeling biologically inspired hair cell sensors for flow control applications. We model the sensor output as well as the effect of the sensors on the flow and present numerical results.

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MS89

Mesh Independence for a Newton-Based Ricatti Solver

In this paper we consider the convergence of the infinite dimensional version of the Kleinman-Newton algorithm for solving the algebraic Riccati operator equation associated with the linear quadratic regulator (LQR) problem. In particular, we establish mesh independence for this algorithm. The importance of dual convergence and preservation of exponential stability (POES) with regard to strong convergence of the functional gains and mesh independence of the algorithm are discussed. These results are applied to systems governed by delay equations and numerical results are presented using different approximation schemes.

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MS90

Recent Advances in Nonlinear Model Predictive Control

The paper reports on advances in real-time computation of constrained closed-loop optimal control, in particular the special case of NMPC, of large DAE systems arising e.g. from semi-discretization of instationary PDE. One of the basic features of the new approach is that in each iteration of the optimization process, new process data are used. In real experiments for distillation columns it is orders of magnitude faster than off-line optimization-based approaches. The approach can be further drastically accelerated by special algorithmic schemes for on-line feasibility and optimality improvement.

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MS90

Mesh Adaptivity in Constrained Optimal Control

An a posteriori analysis of adaptive FEM for control constrained optimal control of elliptic PDEs is presented. The error analysis is based on residual-type estimators consisting of edge and element residuals, as well as data oscillations. Algorithmically, a bulk criterion is invoked and a greedy algorithm is applied during the refinement process. Numerical results are discussed including the case of lack of strict complementarity.

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MS90

Microfluidics: Where Optimization Hides?

We gather here some of our experiences in the numerical simulation, optimization and control of microfluidic devices. This is a collaborative work between Stanford Microfluidic Laboratory in the United States and Montpellier Mathematics and Modelling Institute in France. Microfluidics develop nanometric characteristics length with a large range of variation for both physical coefficients and variables. These make their calculation complex. Sometimes, the quantities are not detectable by the available measuring apparatus and modelling and simulation are valuable tools to develop approaches to make them detectable. Solutions discovered after modelling, simulation and optimization are often non intuitive and allow in certain cases a return on physical modelling, in particular by identifying the significant points in a coupled ensemble.

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MS90

On Level Set Regularization for Highly Ill-Posed Distributed Parameter Estimation Problems

We consider level set regularization for distributed parameter inverse problems that involve elliptic forward PDEs. For this we propose a dynamic regularization method that may be viewed as a regularized Gauss-Newton applied to the output least squares formulation. Our stopping criterion for the iteration does not involve knowledge of the true solution, and normally less than 10 iterarions suffice. We also propose a new, quartic, non-local regularization term that penalizes flatness and produces a smooth level set evolution. Two numerical test cases are considered: a potential problem and the classical EIT/DC resistivity problem.

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MS91

Prediction and Hindcasting of Hurricane Storm Surges

Coastal hydrodynamic models can be used to study many phenomena, including hurricane storm surges, sediment transport, contaminant transport, and circulation/wave coupling. Circulation in shallow coastal waters is complicated by highly irregular geometries, wetting and drying, and near-shore/continental shelf/deep water coupling, which results in flows exhibiting multiple scales. A number of finite element-based simulators have been developed over the past twenty years for modeling these complex flows. One of the more successful of these models is the ADCIRC (Advanced Circulation) Model. We will describe the evolution of this model and the application of it to hindcasting and forecasting storm surges along the southern Louisiana and Texas coasts.

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MS91

Adaptive and Implicit High Order Methods for Two-Phase Flow

Because of the highly heterogeneous geological structure of the subsurface, there is a need for reliable numerical methods that would model flow and transport in non-uniform porous media. We present high order numerical methods for solving the incompressible two-phase flow problem. The incompressible flow of a wetting phase and a non-wetting phase is mathematically modelled by a system of nonlinear partial differential equations derived from the conservation of mass and momentum equations for each phase. In this work, the capillary pressure, i.e. the difference between the phase pressures, is modeled by the Brooks-Corey equations. We consider one sequential and two implicit pressure-saturation formulations for two-phase flow. The primary variables are approximated by discontinuous polynomials of different degrees. We present slope limiting techniques on non-conforming meshes for the sequential approach. For the fully implicit approaches, we show that no slope-limiter or upwinding techniques are needed. Numerical simulations obtained for benchmark problems for homogeneous and heterogeneous media are presented.

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MS91

An Efficient Approach for Estimating Subsidence in Heterogeneous Geological Formations

We consider the estimation of the subsidence produced as a consequence of the pore pressure reduction in oil and gas reservoirs. It is assumed that the reservoir is immersed into a semi-infinite homogeneous medium and has a pore pressure and elastic modulii different than those of its surroundings. The displacement around the reservoir is then put in the form of an integral equation by using the half-space Greens function. Solutions to the integral equation were obtained for some limiting cases. A more general solution was obtained by using quadratures and solving the resulting linear set of equations.

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MS91

Eulerian-Lagrangian Particle-in-Phase Methods for Multiphase Multicomponent Transport

The Eulerian-Lagrangian localized adjoint method (ELLAM) was originally developed for linear advection-diffusion equations. It has no CFL condition, handles all kinds of boundary conditions rigorously, is fully mass-conservative, and its Lagrangian step symmetrizes the advection-diffusion operator. We present here a natural adjoint formulation that extends ELLAM to multiphase multicomponent flows with nonlinear fluxes. This is based on a physical interpretation of the dual adjoint operator as a propagator of mass-carrying particles, in contrast to the wave-propagating primal direct operator. The adjoint operator is linear, so that its space-time characteristics do not intersect, shocks do not form, and particles do not disappear. This makes the dual framework, which is applied to each phase of a multiphase flow, substantially more tractable computationally. All of these concepts are illustrated in some examples and in the discretization of a compositional model.

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MS92

Stable, High-Order Methods for Bounded-Obstacle Scattering

A stable and high-order numerical method for solving the Helmholtz equation on two- and three-dimensional domains exterior to a bounded obstacle will be described in this presentation. The method is based on a boundary perturbation technique ("Transformed Field Expansions") coupled with a well-conditioned, high-order, spectral-Galerkin solver. The method is further enhanced with numerical analytic continuation implemented via Pade approximation. Numerical results will be presented to show the accuracy, stability, and versatility of our new method.

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MS92

Title Not Available at Time of Publication

Abstract not available at time of publication.

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MS92

Advances in Wave Propagation with the Discontinuous Galerkin Method

Two important features relating to the discontinuous Galerkin (DG) method for wave propagation will be discussed. Recent investigations of the spectral properties of the discrete DG operators have revealed important connections with their continuous Galerkin counter parts. Theoretical and numerical results will be shown which demonstrate the correct asymptotic behavior of these methods and controls spurious solutions under mild assumptions. Given the suitability of DG for solving Maxwell's equations and their ability to propagate waves over long distance, it is natural to seek effective boundary treatments for artificial radiation boundary conditions. A new family of far field boundary conditions will be introduced which gracefully transmit propagating and evanescent components out of the domain. These conditions are specifically formulated with DG discretizations in mind, however they are also relevant for a range of numerical methods.

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MS92

Efficient Collocational Approach for Parametric Uncertainty Analysis

A numerical algorithm for effective incorporation of parametric uncertainty into mathematical models is presented. The uncertain parameters are modeled as random variables, and the governing equations are treated as stochastic. The solutions, or quantities of interests, are expressed as convergent series of orthogonal polynomial expansions in terms of the input random parameters. A high-order stochastic collocation method is employed to solve the solution statistics, and more importantly, to reconstruct the polynomial expansion. While retaining the high accuracy by polynomial expansion, the overall algorithm is straightforward to implement as it requires only repetitive deterministic simulations. Error analysis is conducted and numerical examples are presented.

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MS93

A Schur-Based Algorithm to Compute the Smallest Eigenvalue of Symmetric Positive Definite Toeplitz Matrices

The problem of computing the smallest eigenvalue and corresponding eigenvector of symmetric positive definite Toeplitz matrices is of considerable interest in signal processing. All the iterative algorithms developed so far require to compute the solution of a linear system with a Toeplitz coefficient matrix. The latter problem is solved via the Levinson algorithm. In this talk we describe a completely different approach. Each step of the new iterative algorithm yields a lower approximation of the smallest eigenvalue of the involved symmetric positive definite Toeplitz matrix, relying on the generalized Schur algorithm. The complexity and the numerical results are comparable to those obtained by the other algorithms available in the literature.

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MS93

A Generalized Isometric Arnoldi Algorithm

This talk describes a generalization of the isometric Arnoldi algorithm that orthogonalizes a sequence of the form $x_k = Ax_{k-1} + y_k$ where y_k lies in a fixed low dimensional subspace for each k. Particular cases include the columns of Toeplitz-like and block Toeplitz-like matrices. The algorithm has the same relation to the generalized Schur algorithm as the isometric Arnoldi algorithm has to the Schur algorithm.

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MS93

Generalized Vandermonde Matrices Associated with Chebyshev Polynomials

We present some families of generalized Vandermonde matrices that are constructed as a Gram matrix of a basis of the space of polynomials of degree at most n and a basis of the dual space. We consider Lagrange matrices, and their derived matrices, which are determined by two sets of $n+1$ pairwise distinct points in the plane. Such matrices transform the vector of values of an arbitrary polynomial p (of degree at most n), on one of the sets, into the values of p (and its derivatives) on the other set. We also consider Chebyshev-Vandermonde matrices that are closely related to discrete trigonometric transforms.

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MS93

Superfast Multifrontal Method for Large Structured Linear Systems of Equations

We develop a superfast direct method for solving disretized linear systems from certain PDEs such as eliptic equations. The method uses nested dissection ordering in the multifrontal method. For those systems the update and frontal matrices in this procedure have certain low rank properties which can be efficiently exploited by Hierarchically Semi-Separable (HSS) matrix structures(Chandrasekaran, Gu, etc.) A set of efficient HSS operations are proposed. These lead to a superfast multifrontal method with cost nearly linear to the matrix dimension.

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MS94

Iterative Operator Splitting Methods As Effective Decomposition Methods For Multiphysics Problems: Theory And Application

We present a class of iterative operator splitting methods as effective decomposition methods for evolution equation related to multiphysics problems. The advantage of decoupling complicate physical processes to local adaptive simpler physical processes motivates us to combine the wel-known classical operator-splitting methods with iterative techniques to obtain iterative operator-splitting methods. We present the stability- and consistency analysis of the iterative operator splitting methods. The numerical experiment are done for stiff systems of linear and nonlinear convection-diffusion-reaction equations. Finally, we discuss the benefits of our iterative methods and the extention to non-smooth and discontinuous applications.

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MS94

Linearly Implicit LOD Methods For ReactionDiffusion Systems

We present Locally One-Dimensional (LOD) methods for the reaction diffusion systems in which the non-linear terms are treated in a linearly implicit manner that avoids necessity of iterating at each time step while maintaining stability properties of corresponding one dimensional operator. The elegant extrapolation methods of LawsonMorris, and Verwerde-Vries are couched into this technique and are shown to be computationally efficient for nonlinear problems. A method based on rational approximation with real distinct poles having a positivity property is highlighted. Numerical results are presented on reactiondiffusion systems including problems in enzyme kinetics and population ecology.

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MS94

Higher-Order Operator Splitting Methods And Their Application In Quantum Computers

In this talk, I will discuss some higher-order operator splitting methods developed by Ewan Stewart and myself. The discussion will cover the derivation of the methods and some of their advantages, including the fact that they work for an arbitrary number of non-commuting operators. I will then go on to discuss some applications in quantum simulations and control methods for quantum computers.

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MS94

On Growth Factors Of The LU, Cholesky, And Modified Gram-Schmidt Factorizations In Splitting

Growth factors play a central role in studying the stability and roundoff estimates of matrix factorizations. It has become evident that growth factors for the LU and modified Gram-Schmidt factorizations grow exponentially with the dimensions of the matrices used in the splitting method. In this talk, we will define row-wise growth factor for the LU factorization, and derive the upper bounds of these factors for the LU factorization which are related to the condition numbers of sub-matrices of the matrix. We will also obtain two kinds of upper bounds of the growth factors for the MGS algorithm on a matrix, or a row scaled matrix, and then extend the analysis to the MGS-like algorithms.

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PP0

AWM Poster: A Mathematical Model Of Network Dynamics Governing Sleep-Wake Patterns In Mice

Behavioral states of wake, sleep, REM sleep, and the transitions among them, are regulated by a network of neurons in the brainstem and hypothalamus. We model network dynamics using coupled relaxation oscillators. The fast-slow nature of the network captures fast transitions between states and leads to canard-like behavior. We identify mechanisms of transition by analyzing a sequence of reduced systems obtained using combinations of fast-slow and dominant scale techniques.

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PP0

AWM Poster: A Hörmander-type Pseudo Differential Calculus on the Heisenberg Group

A general overview of pseudo differential operators and calculi will be presented, including an approach which allows working on homogeneous groups. Using convolution operators, in the spirit of the Calderón-Zygmund theory, the existence of a Hörmander-type pseudo differential calculus will be proved for the Heisenberg group, notable for being a non-commutative, non-compact Lie group, as well as for its connections with the theory of image processing.

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PP0

AWM Poster: An Edge-Flame in a Mixing Layer

The behavior of an edge-flame in a mixing layer was studied numerically. Using a reaction diffusion model we considered a system in which fuel and oxidizer are separated by a thin plate and flow into the system with a prescribed uniform flow. At the end of the plate fuel and oxidizer mix and an edge-flame is sustained at some distance from the plate. We allowed for the conduction of heat along the plate and consider its effect on the flame stand off distance. We also examined the effect of varying the Lewis numbers for both the fuel and oxidizer and the effect of both lean and rich conditions, by varying the initial mixture strength. These parameters affect the flame shape, location, and its distance from the separating plate.

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PP0

AWM Poster: Mathematical Modeling of Cellular Signaling in Macrophages: Understanding Pathways

Our goal is the construction of a comprehensive mathematical model for the uridine 5-diphosphate signaling pathway in the macrophage, a type of white blood cell. The mathematical model currently includes a system of nonlinear ODEs that describe the major pathway components, with an emphasis on the production and degradation of diacylglycerol, a cellular second messenger molecule which plays an important role in initiating various changes in cell behavior. Modeling techniques, challenges, and computational simulations will be presented.

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PP0

AWM Poster: Wellposedness and Control of Nonlinear Structural Acoustic Interactions

The project pertains to the mathematical analysis of solutions to nonlinear systems of partial differential equations modeling structural acoustic interactions. An acoustic chamber surrounded by an active plate or wall is considered. A nonlinear model which accounts for thermal effects in the wall and dispenses with the need for structural damping of the wall is studied. Issues such as global existence and uniqueness of nonlinear solutions, their stability and control are in the main focus of the research.

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PP0

AWM Poster: Vacuum Formation in Multi-Dimensional Compressible Flows

It is well known that vacuum formation can occur for inviscid compressible flows. However, for viscous compressible flows, governed by the Navier-Stokes equations, vacuum formation in the multidimensional case is an open question. The analytic difficulties associated with this problem translate into numerical difficulties requiring the use of a highly accurate method. Using a spectrally accurate collocation method, we show that vacuum formation does occur under certain conditions.

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PP0

Analyzing Methods of Water Allocation Through Simulation and Optimization

Regions can establish water markets, the buying and selling of water, as a strategy to efficiently allocate water and prevent water scarcity. Each municipality within a region wants to meet their water demand with minimum cost. A stochastic water market simulation for one municipality creates a cost-based solution surface with high-frequency, low-amplitude noise. We use the optimization technique called implicit filtering to investigate scenarios to aid in water management decisions.

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PP0

A Block Quasi-totally Pivoted LU Decomposition

The totally pivoted LU decomposition is the most stable among all LU-like factorizations, but unfortunately also computationally expensive, and not amendable to exploit level 3 BLAS operations. In this contribution, we derive a block organized LU factorization, in which at each step of the algorithm a totally pivoted LU decomposition is applied to a sub-block of the current matrix. An optimal exploitation of the matrix-matrix products results in a significantly improved performance.

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PP0

Moment-of-Fluid Interface Reconstruction (poster)

A new mass-conservative interface reconstruction method is presented. Unlike volume-of-fluid methods, which calculate the interface location from the volumes of the cell fractions occupied by different materials, the new algorithm localizes the interface based on both volumes and centroids of the cell fractions. The normal of the linear interface in each mixed cell is determined by fitting the centroid of the fraction behind to the reference centroid. This results in a second order accurate interface approximation, which is shown to be more accurate than the volume-of-fluid counterparts.

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PP0

SIAM-DW: The Method of Images for Regularized Stokeslets

Abstract not available at time of publication.

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PP0

AWM Poster: Improving Forecasts for Chaotic Physical Processes by Improving Initial Conditions

Accurate estimates of the initial atmospheric state are necessary for accurate weather forecasts. Initial condition estimates combine forecast and observation information relative to their uncertainties. Algorithms estimating the initial conditions at meteorological centers (e.g. PSAS) assume a constant forecast uncertainty. The LETKF algorithm uses ensembles to evolve forecast uncertainties efficiency. We apply LETKF and PSAS to the NASA weather model, fvGCM. LETKFs estimate of the initial conditions has fewer errors than those of PSAS.

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PP0

AWM Poster: Front Dynamics of a Singular Perturbation Non-smooth Ignition Process

A proton exchange membrane (PEM) fuel cell is a device capable of generating electricity directly by means of two electrochemical reactions which take place at the proton exchange membrane/catalyst interface at low temperatures. Recent experimental work has shown that PEM fuel cells can exhibit long term transients, hysteresis, and long period oscillations when run under fixed load with unhumidified gases. We recover the experimental hysteresis and investigate the stability of a simplified model which has a simple but discontinuous nonlinearity. We study the nonlinear stability of the model which follows from the decay

of linear semigroup via a simple, but effective, renormalization group argument.

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PP0

Numerical Study of Two-Phase Flow on Locally Refined Meshes

For geological heterogeneities, methods are needed for modelling flow and transport in non-uniform porous media. We present a non-symmetric interior penalty Galerkin formulation of two-phase flow equations, based upon PDEs derived from mass conservation and Darcy's Law, with closure by Brooks-Corey equations. The pressure and saturation equations are decoupled and solved sequentially. Also considered are proposed space and time adaptivity techniques; slope limiters for nonconforming meshes; numerical examples of heterogeneous media in 3D.

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PP0

Approximation of the Singularity Curve of a Piecewise Constant Function of Two Variables by Its Fourier-Jacobi Coefficients

A new method is considered to approximate the singularity curve of a piecewise constant function of two variables by means of its Fourier-Jacobi coefficients. The method is based on the technique suggested by the author for recovering the locations of discontinuities of a piecewise smooth function of one variable. In addition, some numerical examples are presented.

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PP0

Integrate-and-Fire Neurons Coupled by Gap Junctions

In integrate-and-fire models of neurons, the suprathreshold portion of the spike is not usually modeled explicitly. However, when neurons are coupled by gap junctions, this portion of the spike is crucial. When modeling neurons coupled by gap junctions using integrate-and-fire models, one must therefore introduce a correction accounting for the suprathreshold portion of the spike. We examine to which extent the details of this correction matter for network behavior.

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PP0

Efficient Matrix Formalism for Power Series Solutions of the Boundary Value Problems for Hyperbolic Equations

Matrix formalism for finding power series solutions of the main BVP for a hyperbolic PDE is developed. As an example, classic Riemann, Cauchy, and mixed problem for the telegraph equation are solved. Surprisingly, this leads to explicit solutions in terms of generalized hyperbolic functions. Application of these results to a two-dimensional technological problem in plasticity is outlined.

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PP0

Adaptive Temporal Integration of Odes with Interval Computations

The area of Interval Computations is of growing interest for rigorous and error bounded computations. By using interval arithmetic routines in the Matlab toolbox Intlab, error bounds can be propagated throughout an algorithm to yield reliable enclosures of solutions. We examine the use of interval arithmetic applied to adaptive temporal integration of stiff ODEs and solutions to nonlinear systems.

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PP0

Regularized Elastic Collision Operators for High Energy Electron Transport

High energy electrons interact with matter through Coulomb forces which generate sharply varying energy-loss and angular deflection collision operators and result in inefficient Monte Carlo simulation. A procedure to construct approximate but accurate regularized collision operators is presented which relies on Green's functions and moment-preserving constraints to smooth out singularities. Numerical results demonstrating accuracy and efficiency will be presented.

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PP0

Computer Simulation and Experimental Rheology of Pharmaceutical and Cosmetic Products

Applying the principles of rheology to pharmaceuticals, foods, personal care, and plastics industries can reduce cost, develop new products, improve product properties, and accelerate products to market. Rheology lies at the crossroads of physics, chemistry, mathematics, biology, and engineering. In this presentation we introduce experimental and mathematical modeling concepts of rheological problems via (i) basic terminologies and interpretation of rheological response using pharmaceutical products and basic principles for formulation of pharmaceutical suspensions and emulsions of interest (ii) fundamental rheological properties such as using oscillatory and steady state fluid flow by appropriate constitutive equations using generalized Maxwell, Casson, Carrue, and Herschel Buckley model for viscoelasticity. Numerical simulation of material deformation and flow; and application of rheological information to solve process and performance problems

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PP0

Adaptive Grid Methods for Q-Tensor Theory of Liquid Crystals

This poster illustrates the use of adaptive grid methods for solving PDE problems in Q-tensor theory of liquid crystals. We will present the results of an initial study using some simple one-dimensional test problems which illustrates the feasibility of applying adaptive grid techniques in such situations. We describe how the grids are computed using an equidistribution principle, and investigate the comparative accuracy of various grid strategies, both theoretically and via a set of numerical examples.

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PP0

The Power of SLI Arithmetic

A fast and reliable C++ implementation of a hybrid system based on the Symmetric Level-Index number representation will show you the power of SLI arithmetic. It could release you from fighting with overflow/underflow problems in scientific computations! The poster includes a general introduction to the Symmetric Level-Index system. A little detail of the implementation will be followed by its successful applications to matrix condition number estimation and other examples.

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PP0

The Extended Finite Element Method for Boundary Layer Problems in Biofilm Growth

We present a technique for capturing boundary layer behavior with the eXtended Finite Element Method (X-FEM). Customized enrichment functions, determined by asymptotic analysis near the interface, are incorporated into the function space to better approximate the solution within the boundary layer. We present example problems which confirm the accuracy of the method, and then apply the method to the linearized biofilm growth equations in order to explore the "shadowing" of small colonies by larger ones.

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PP0

Probabilistic Domain Decomposition Solution of Elliptic Equations on Polygonal Domains

A probabilistically induced domain decomposition method, recently tested for boundary-value elliptic problems on a unit square, is applied to the case of rather general two-dimensional domains. These have been chosen in the form of polygons, since polygons may approximate very general domains, encountered, e.g., in a number of engineering problems, provided that they have a sufficiently large number of sides. One of the key-point is approximating accurately the "first exit times" and points, which task requires now some more are and work.

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PP0

A Comparison of the Extended Finite Element Method with the Immersed Interface Method for Elliptic Equations with Discontinuous Coefficients and Singular Sources

The authors compare the Immersed Interface Method (IIM) with the eXtended Finite Element Method (X-FEM) for elliptic equations with singular sources and discontinuous coefficients. The IIM has been compared favorably with competing methods. These methods are of particular interest because they allow for the solution of elliptic equations with internal boundaries on non-conforming meshes. In the context of moving interface problems, emphasis is placed on accuracy of solutions and their normal derivatives on the interface.

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PP0

AWM Poster: Patterns of Synchrony in Lattice Dynamical Systems

By using the theory of coupled cell systems developed by Stewart, Golubitsky, Pivato and Torok, we consider patterns of synchrony of lattice dynamical systems. Roughly speaking, a pattern of synchrony is a coloring in which two nodes with the same color if their corresponding dynamics are synchrony for all the time. We classify two-color patterns of synchrony of four kinds of lattice dynamical systems (square and exagonal lattice differential equations with nearest neighbor (NN) coupling and with nearest and next nearest neighbor (NNN) couplings). We show that there are an infinite number of patterns of synchrony of the systems with NN coupling, and all these patterns can be generated from a finite number of distinct patterns. However, there are only a finite number of patterns of synchrony of the systems with NNN coupling, and all patterns are spatially periodic. We also prove that equilibria associated to each such two-color pattern can be obtained by codimension one synchrony-breaking bifurcation from a fully synchronous equilibrium. By using a notion of 'window' (a finite region of a lattice that determines the whole pattern of the lattice), we show that for each k, there are only a finite number of k-color patterns of synchrony of square (*resp.* hexagonal) lattices with NNN architecture, and every k-color pattern of synchrony is spatially periodic. The techniques we developed to prove periodicity and finiteness can be applied to other lattices as well.

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PP0

AWM Poster: Three Dimensional Computational Model of Water Movement in Plant Root Growth Zone

Primary plant root growth occurs in the 10 mm root tip segment where cells expand by stretching the rigid cell wall that constricts their growth. Silk and Wagner (1980) provided an osmotic root growth model to describe this process. Their theory is expanded to a three-dimensional model with the addition of point source terms. This three-dimensional point source model is examined in terms of current plant physiology measurements which results in suggestions for future work.

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PP0

AWM Poster: European Option Pricing for a Stochastic-Volatility Jump-Diffusion Model

An alternative option pricing model is proposed, in which the underlying stock prices follow a compound stochastic-volatility jump-diffusion (SVJD) process with log-uniformly distributed jump amplitudes. Fourier transforms are applied to solve the problem for risk-neutral European option pricing under this model. The numerical implementation of pricing formulas is accomplished by both fast Fourier transforms (FFTs) and more highly accurate discrete Fourier transforms (DFTs) for verifying results and for different output.

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PP0

AWM Poster: Computational Studies of Morphogen Gradients

Concentration gradients of morphogens are known to be instrumental in cell signaling and tissue patterning. A recent study shows that Dlp somatic cell clones disrupt smooth gradient of extra cellular Wg, producing ectopic expression of Wg target genes. We constructed a mathematical model to understand the mechanisms responsible for the observed phenomena and the interactions involved in this complex biological system. The model consists of a system of 2D reaction-diffusion equations. Due to the biological complexity, the system is extremely stiff. Thus, we developed a new class of semi-implicit schemes which removes both time-step constraints on diffusion and reaction terms. Direct numerical simulations showed that the new schemes are efficient, robust and accurate.

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