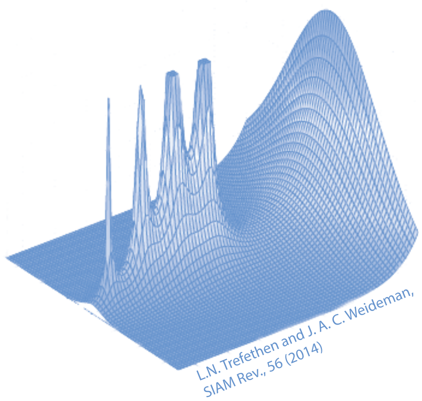
AN16-LS16 Abstracts

2016 SIAM ANNUAL MEETING

JULY 11-15, 2016



THE WESTIN BOSTON WATERFRONT
BOSTON, MASSACHUSETTS, USA

SIAM Conference on the

Life Sciences

July 11-14, 2016

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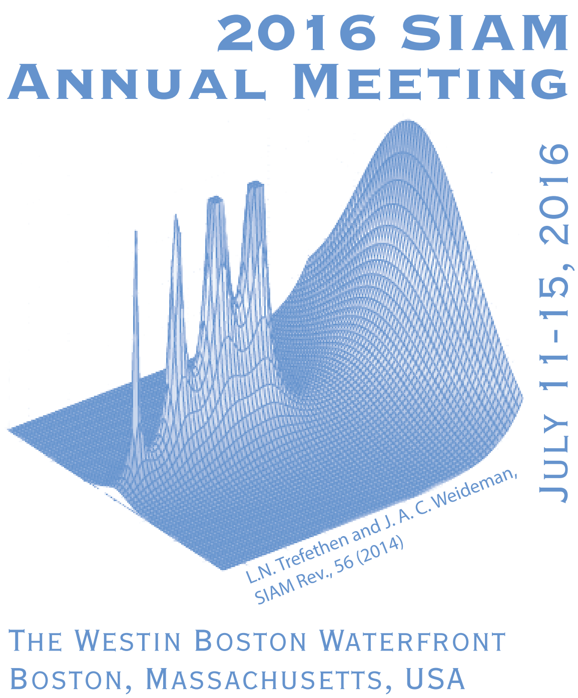

SP1

AWM-SIAM Sonia Kovalevsky Lecture - Biofluids of Reproduction: Oscillators, Viscoelastic Networks and Sticky Situations

From fertilization to birth, successful mammalian reproduction relies on interactions of elastic structures with a fluid environment. Sperm flagella must move through cervical mucus to the uterus and into the oviduct, where fertilization occurs. In fact, some sperm may adhere to oviductal epithelia, and must change their pattern of oscillation to escape. In addition, coordinated beating of oviductal cilia also drives the flow. Sperm-egg penetration, transport of the fertilized ovum from the oviduct to its implantation in the uterus and, indeed, birth itself are rich examples of elasto-hydrodynamic coupling. We will discuss successes and challenges in the mathematical and computational modeling of the biofluids of reproduction. In addition, we will present reduced models that evoke intriguing questions in fundamental fluid dynamics.

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SP2

The John von Neumann Lecture: Satisfiability and Combinatorics

The Satisfiability Problem, which asks whether or not a given Boolean formula can be satisfied for some values of its variables, has long been thought to be computationally hopeless. Indeed, SAT is the well-known ”Poster Child” for NP-complete problems. But algorithmic breakthroughs have made it possible for many important special cases of the problem to be solved efficiently. Industrial-strength ”SAT solvers” have become a billion-dollar industry, and they play a vital part in the design of contemporary computers. The speaker will explain how the new SAT technology also helps us to solve a wide variety of problems that belong to combinatorial mathematics.

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SP3

W.T. and Idalia Reid Prize in Mathematics

Not available at time of publication.

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SP4

I. E. Block Community Lecture: Toy Models

Would you like to come see some toys? ’Toys’ here have a special sense: objects of daily life which you can find or make in minutes, yet which, if played with imaginatively, reveal surprises that keep scientists puzzling for a while. We will see table-top demos of many such toys and visit some of the science that they open up. The common theme is singularity.

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JP1

Spatio-temporal Dynamics of Childhood Infectious Disease: Predictability and the Impact of Vaccination

Violent epidemics of childhood infections such as measles provide a particularly clear illustration of oscillatory ’predator-prey’ dynamics. We discuss limits on the predictability of these systems, both in the era before vaccination and at present, where vaccine hesitancy limits the effectiveness of vaccination programs in many countries. We also discuss the impact of viral evolution on predictability and the design of vaccination programs, with particular reference to influenza and rotavirus.

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CP1

Analysis of Block Methods for Toeplitz Matrices

Toeplitz matrices and matrices from related matrix algebras arise in a variety of applications including signal processing and partial differential equations. The analysis of iterative solvers for linear systems is usually based on studying the generating symbol of the iteration matrix. Block methods can be studied using proper decompositions of the matrices, resulting in analyses that fit in the established framework used to analyze non-blocked methods. These techniques will be presented in this talk.

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CP1

A Feast Eigenvalue Algorithm Without Solving Linear Systems

The FEAST Eigenvalue algorithm uses a shift-invert strategy that requires solving multiple linear systems in the complex plane. Similarly to other shift-invert algorithms, solving the linear systems represents the most challenging part of the computation. We present an innovative modification of FEAST that finds interior eigenpairs without solving linear systems, instead using only a few iterations of iterative refinement per subspace update, thus removing the need for using matrix factorizations or preconditioner matrices.

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CP1

Combining Krylov Subspace Recycling with Recycling Preconditioners for Sequences of Linear Sys-

tems

Preconditioners are generally essential for fast convergence of iterative solvers. For sequences of systems, it may be advantageous to recycle (update and reuse) preconditioners. Recycling Krylov subspaces from previous systems is a complementary method for reducing computational cost. We examine the combination of recycling subspaces with recycling preconditioners, providing theoretical and numerical analysis. Applications include model reduction, tomography, and others.

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CP1

Neighbor Discovery for Algebraic Multigrid and Matrix Migration

The idea of a neighbor — processors to whom point-to-point messages get sent/received — is core to MPI-based parallelism. Finding those communication patterns requires neighbor discovery, which can be quie expensive. We will focus on two computational kernels involved in algebraic multigrid — migration of sparse matrices between processors and sparse matrix-matrix multiplication. We will show that for these kernels, passing additional information during point-to-point communication can allow one to perform neighbor discovery more efficiently.

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CP1

Heavy Ball Minimal Residual Method for Least-Squares Problem

The heavy ball minimal residual (HBMR) method is presented for solving overdetermined least-squares problem $\|Ax - b\|_2$, where A is a sparse matrix. HBMR method seeks optimal approximate solutions of the least- squares problem by minimizing the residual norm $\|A^T r\|_2$ over both the Krylov subspace obtained by the restarted Golub-Kahan bidiagonalization process and the information of the Krylov subspaces in the previous cycles. Numerical experiments are reported to show the advantages of the HBMR method.

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CP2

New Insights into Scaling Laws: The Lavalette Distribution and Its Properties

We introduce a novel family of probability densities which proves useful in modelling the size and rate distributions in various phenomena. This law, that we call *Lavalette distribution*, is derived analitically from a generalization of power laws. We propose a model of random variable subtraction that lead to this distribution. We illustrate the utility of the Lavalette distribution in several dataset and discuss estimation and goodness of fit methods.

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CP2

Optimizing Radioactive Contamination Monitoring Using Utility Functions in a Bayesian Network

After an incident involving radionuclides release, the level of radioactive contamination of individuals is assessed from results of bioassay monitoring. Such retrospective assessment is prone to uncertainty which Bayesian methods are well-adapted to evaluate. An algorithm based on a Bayesian network (BN) providing an initial quantification of the contamination and its associated uncertainty was developed to optimize bioassay monitoring. The best follow-up program is then determined through a prospective utility function integrated in the BN.

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CP2

Modeling Extreme Weather Events

The 2016 Blizzard brought disastrous outcomes to the Northeastern U.S. Using extreme value analysis to analyze NYCs historical daily extreme snowfall data up to the 2006-2007 winter, we will determine if predicting the Blizzard was reasonable. Initial analysis shows that time-independent extreme value models did not predict the Blizzard, suggesting models need to take climate changes into account. We also will use data up to January 2016 to assess return levels for future extreme events.

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CP2

Gaussian Approximation for Transition Paths in Molecure Dynamics

We are interested in determining the most likely transition paths in molecular dynamics. The Onsager-Machlup approach, based on maximal probability leads to transitions that exhibit unphysical characteristics. We propose a method based on Kullback-Leibler minimization for finding the best Gaussian approximation to a path-space measure. Low temperature limit of the Gaussian approximation is studied via Γ convergence. Our approach removes the unphysical effects of Onsager-Machlups approach and recovers the Freidlin-Wentzell theory in zero temperature limit.

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CP2

Large Deviations for a Stochastic Burgers' Equation

We prove the large deviations principle (LDP) for the law of the solutions to a stochastic Burgers' equation in the presence of an additive noise. Our proof is based on the weak convergence approach.

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CP2

On a Storage Allocation Model with Finite Capacity

We consider a storage allocation model with a finite number of ranked primary and secondary storage spaces. Each item arrives according to a Poisson process, takes the lowest ranked available space, and occupies a space for an exponentially distributed time. We study the joint distribution of the numbers of occupied primary and secondary spaces in the steady state. We obtain explicit expressions for the joint distribution and the marginal distribution of the occupied secondary spaces.

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CP3

Experiences with SeeMore: A 256-Node Kinetic Parallel Computing Cluster

SeeMore is an award-winning, 256-node cluster of Raspberry Pi computers sponsored in part by the National Science Foundation. The system is a kinetic sculpture where nodes move in response to computational demands. In this presentation I will share the conception, design and use of SeeMore to inspire and educate audiences on the topic of parallel computational thinking at the 2015 International Makers Faire and the 2016 U.S. Science and Engineering Festival.

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CP3

Efficiency of Stochastic Simulations in Chemical Kinetics

I will analyze and theoretically compare the complexity of simulation strategies for continuous time Markov chains, often a bottleneck in biochemical kinetics and cell biology. I will look at Monte Carlo with exact simulation and with tau-leaping, Euler on a diffusion approximation and recent multilevel Monte Carlo versions. I will give practically relevant asymptotic results and also flag up some pitfalls that must be avoided in this type of study.

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CP3

Fast Multipole Preconditioner for Direct Numerical Simulation of Flows Past An Airfoil

We use the Fast Multipole Method, originally developed as an N-body solver, as a preconditioner for sparse matrices arising from elliptic PDEs discretizations by equipping it with boundary integral capability for satisfying conditions at finite boundaries and by wrapping it in a Krylov method. We demonstrate the potential of the FMM-preconditioner by applying it to the pressure equation within a 4th order incompressible Navier-Stokes equation for direct numerical simulation of flows past an airfoil.

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CP3

Numerical Algorithms for Scalable High-Performance Electronic Structure Calculations

We introduce new computational and algorithmic paradigms that can significantly improve the efficiency of existing methodologies used in first-principle electronic ground state and excited states calculations of complex molecular systems and nanostructures. Our modeling framework benefits from well-suited combinations of numerical methods that can both exploit the linear scaling capabilities of real-space mesh techniques, and the hierarchical parallelization strategy offered by the FEAST eigenvalue solver. Specific implementations details, along with performance results, will be discussed.

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CP3

High Resolution Simulation of Coupled Pore-Continuum Flow and Transport in Fractured Subsurface Materials

The response of shales to perturbations from concurrent hydrodynamic, mechanical and chemical stressors is a coupled mesoscale behavior that is not well understood or predictable, yet critical to understanding subsurface problems such as safe carbon storage for sequestration and fracture-induced oil and gas extraction. We present results from first-ever resolved flow in low permeability subsurface materials such as shale. This work is based on the application code Chombo-Crunch which models pore to continuum flow and transport in subsurface materials at unprecedented resolution. Our algorithmic approach is adaptive, finite volume methods based on embedded boundaries which allow for explicit resolution of reactive surface area at the pore scale and coupling at pore-continuum interfaces. The code has been validated by reactive transport experiments and is scalable up to 256K CPU cores.

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CP4

Nonconvex Algorithms for Geosounding Inversion

Tikhonovs regularization method is the standard technique applied to obtain models of the subsurface conductivity distribution from electric or electromagnetic measurements.

$$U_T(m) = \|F(m) - d\|^2_{\mathcal{H}} + \lambda P(m). \quad (1)$$

The second term correspond to the stabilizing functional, with $P(m) = \| \bigtriangledown m\|^2_{\mathcal{M}}$,the usual approach and λ the regularization parameter. Due to the roughness penalizer inclusion, the model developed by Tikhonov's algorithm tends to smear discontinuities, a feature that may be undesirable. An important requirement for the regularizer is to allow the recovery of edges, and smooth the homogeneous parts. As is well known, Total Variation (TV) is now the standard approach to meet this requirement. Recently, Wang et.al. proved convergence for alternating direction method of multipliers in nonconvex, nonsmooth optimization. In this talk we present algorithms for model recovering of Geosounding data based on nonsmooth, nonconvex optimization, providing for better model recovery than TV.

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CP4

A Partially Collapsed Gibbs Sampler for Computing the Point Spread Function of An X-Ray Imaging System

In quantitative radiography it is essential to deconvolve the system impulse response out of measured imagery in order to compute absolutely correct values of object properties like densities or feature locations. For high-energy X-ray systems, it is necessary to experimentally determine the system response – the so-called Point Spread Function (PSF) – by measuring calibration imagery and computing the PSF from the calibration. In this work we present a hierarchical Bayesian model for computing the PSF of an X-ray system from a particular calibration object, a partially collapsed Gibbs sampler for efficiently computing samples from the posterior, and results from a real high-energy system at the U.S. Department of Energy's Nevada National Security Site.

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CP4

Real-Time Computing of Touch Topology via Poincare-Hopf Index

The topological invariants such as the number of connected components or holes in a binary image are informative for pattern recognition such as digits discrimination, but hard to compute in real time. We propose an algorithm that gives a fast way to compute the Euler characteristics by only counting a handful of critical points in the image lattice.

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CP4

Constrained Smoothing Splines on Unit Balls with Application to Optical Coherence Tomography

An interesting problem is the reconstruction of the shape of the biological tissue from Optical Coherence Tomography (OCT) images. The problem is cast as a weighted least squares regression with a penalty on the magnitude of the second derivative (Laplacian) of the surface. The solution is a smoothing spline on a disk domain, which is obtained using a famous result by Kimeldorf and Wahba. We present an application to OCT date from a human eye.

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CP5

The Benefits of Applying Data Mining Algorithms on Medical Data

Data mining can give better results than statistical approach, and it can add greater research depth and breadth specifically when applied on medical data due to the complexity and diversity of collected data sets. Data Mining can provide the methodology and technology to move these comprehensive data into useful information for healthcare decision making. Applying data mining algorithms on state inpatient data resulted in deeper and more accurate information that what statistical methods gave.

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CP5

Leveraging Computationally-Predicted Adverse Outcome Pathways for Optimizing Alternatives to Animal Testing

Replacing animal use for chemical safety testing with in vitro and in silico test methods poses the challenge of how to couple molecular- and cellular-level changes with the adverse outcome observed in vivo. Computationally-predicted adverse outcome pathways (cpAOPs) are a graph-based approach to data integration that leverage the AOP framework, public data repositories, and experimental data. We present how mining cpAOPS facilitates interactive chemical safety test-battery design and accelerates manually-curated AOP development.

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CP5

A Nearest-Neighbor Approach for Fast, Accurate Selection of the Scale Parameter in Gaussian-Kernel Support Vector Machines

We present novel machine learning techniques for efficient selection of the scale parameter in Gaussian-kernel SVM. Unlike the widely-used LIBSVM implementation which uses a fixed grid, our method exploits the geometry of training data and uses the nearest neighbors of a small subset of randomly selected training points to set the parameter value. Extensive numerical experiments show that our method is at least comparable to LIBSVM in terms of classification accuracy, but significantly faster.

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CP5

Mode Reduction Methods for Data Assimilation: Subspace Projection using Koopman Operators

In order to reduce the computational burden of assimilating data into large-scale systems, spectral decomposition methods are used to to define a subspace that reduces the dimension of the problem. In this talk we use a recent decomposition technique based on the Koopman operator and present how it applies to data assimilation methods. We will derive an approximation to the eigenfunctions defined by the Koopman operator that represent the nonlinear behaviour of a dynamical system.

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CP5

Rigorous Model Validation and Certification Via the Ouq Algorithm in 'mystic

In machine learning and data science, the prevalence of parallel computing has stimulated a shift from reduced-dimensional models toward more brute-force methods for solving high-dimensional nonlinear optimization problems. The 'mystic software enables the solving of difficult UQ problems as embarrassingly parallel non-convex optimizations; and with the OUQ algorithm, can provide validation and certification in a UQ context. We discuss how 'mystic can be used for model validation, and demonstrate this in the context of classification.

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CP5

Nonasymptotic Rates in Distributed Learning

We consider the problem of distributed learning where a group of agents repeatedly observe some random processes and try to collectively agree on a hypothesis that best explains the observations. Agents interact in a time-varying directed graph sequence. We propose a distributed learning rule and establish nonasymptotic, explicit, geometric convergence rates. Additionally, for fixed undirected graphs, we provide a protocol which has better scalability with the number network nodes in the network.

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CP6

Numerical Computing with 3D Functions in Chebfun

We present an algorithm for numerical computations involving trivariate functions over a 3D box in the context of Chebfun. Our scheme, which is based on low rank representation through multivariate adaptive cross approximation (MACA), computes a Tucker decomposition of the given function. If the function is periodic in all three variables, then trigonometric polynomials can also be used. Numerical experiments show that our approach can be successfully applied for numerical computing with 3D functions.

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CP6

Spectral Methods for Fractional Differential Equations on the Half-Line with Tunable Accuracy

In this talk, we introduce new Laguerre Petrov-Galerkin spectral methods for fractional differential equations on the half-line. We will demonstrate the tunable accuracy of these methods and the sensitivity of the accuracy due to the tuning parameter using numerical experiments. We also show that these approaches result in more accurate and computationally efficient methods for solving multi-term fractional differential equations on the half-line compared with previously proposed methods.

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CP6

Numerical Solution of Boundary-Integral Equations for Nonlocal Models of Molecular Electrostatics Using Bem++

Biomolecule function and structure is greatly influenced by electrostatic interactions between the biomolecule and surrounding water molecules and dissolved ions. Its been a significant challenge to develop a precise and efficient theoretical approach to investigate biomolecular electrostatics since the topic was first introduced in early 20th century. Nonlocal electrostatics theory has been employed to improve our description of the dielectric function of solvent on small length scales. A system of boundary integral equations has been developed to find electrostatic potentials on surface of solvated molecules, and we report the use of the BEM++ boundary element method library to solve the equations.

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CP6

Approach to Model Acoustic Wave Scattering Using Time Domain Boundary Integral Equations

In aircraft design, there is a need to accurately predict the acoustic scattering by an aircraft body from a given noise source. Numerical techniques for modeling acoustic wave scattering by complex geometries using time domain boundary integral equations will be discussed. Geometries investigated include spheres and flat plates. Scalability of high performance parallel computing will be discussed, and the use of acoustic liners will be considered as a method for absorbing sound of scattering bodies.

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CP6

Chopping a Chebyshev Series

Chebfun and related software projects for numerical computing with functions are based on the idea that at each step of a computation, a function is "rounded' to a prescribed precision by chopping a Chebyshev series at an appropriate point. Designing a chopping algorithm with the right properties proves to be a surprisingly complex and interesting problem. We describe the algorithm introduced in Chebfun Version 5.3 in 2015 and the considerations that led to this design.

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CP6

Numerical Computing in Polar and Spherical Geometries

Synthesizing the double Fourier sphere method with new ideas in low rank approximation, we construct approximants to functions in polar and spherical geometries. Our approach preserves smoothness for functions on the sphere/disk, overcomes issues associated with artificial singularities, is near-optimal in its underlying interpolation, and powers a suite of fast, scalable algorithms for numerical computing. The talk will include demonstrations in the Chebfun software system, where these algorithms are fully implemented and publicly available.

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CP7
Running and Falling: Dynamics on Rough Terrains

We model running as drag-free flight with intermittent ground contact, and use Monte-Carlo methods to study stability on rough terrains. By analyzing the dynamics over one step, we find a single dimensionless parameter that governs the likelihood of falling, and show that falling probabilities are Lévy distributed. Open-loop strategies suffice for stability on piecewise-flat terrains, but anticipatory strategies and feedback control become necessary on realistic terrains with height and slope variations.

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CP7
An Efficient $O(n^2)$ Algorithm for Solving the Dynamic Matching Problem in TFT-LCD Cell Assembly Process

We consider the dynamic matching problem in the cell assembly process for producing TFT-LCD (Thin Film Transistor-Liquid Crystal Display) panel, where two components, TFT array and color filter (CF) substrates are matched to assemble a final product, the LCD display. This component assembly problem is formulated as a mathematical programming model, with the objective to optimize the yield rate in the cell assembly process. In the new formulation, a full size panel is cut into several equal sized sub-panels, based on the selected precut pattern. After the precut, a lexicographic order for the location of (good, defective) displays in each sub-panel is generated. For each precut pattern, a yield matrix for the mating of TFT and CF sub-panels is then constructed. We explore the special structure of this new model and characterize some interesting properties. Based on these findings, efficient algorithms are developed for determining the optimum matching. Computational experiments with different precut patterns and a wide range of batch sizes indicate that the solution procedures are effective and efficient.

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CP7
Null Controllability of a Non-Linear System Governed by a Nonlocal Operator

This paper is concerned with the simultaneous null controllability of a system of two coupled equations governed by a quasilinear nonlocal operator, under constraints on the state. Such a system can be used the context of population dynamics in biology. The control is exerted on a subdomain ω of the bounded open set Ω. We prove that the system is null controllable provided that one of the coefficients of the system is, in absolute value, far from zero in a subdomain of ω.

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CP7
The Stochastic Linear Quadratic Control Problem on Hilbert Spaces: Theory and Applications

We consider the stochastic linear quadratic regulator (SLQ) control problem on Hilbert spaces. The optimal control is given in terms of a Riccati equation. We develop a stochastic treatment of unbounded control action problems arising in a general class of dynamical systems which exhibit singular estimates. In addition, we investigate the numerical treatment of the SLQ problem, convergence of the Riccati operators and methods for solving Riccati equations. We also discuss some applications.

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CP7
Direct Adaptive Control, Direct Optimization

The purpose of this paper is twofold. First is to present a design method to solve a longstanding problem: that of constructing direct adaptive controllers for multivariable linear plants which may have zeros as well as poles in either half of the complex plane. This is of interest mostly to the controls community. Second is to show new results on a method for derivative–free optimization, called the barycenter method, which was previously presented at the SIAM OP14. The new results show that the method is particularly suitable for adaptive control, as well as for other direct optimization problems.

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CP7
Boundary Observation in Shape Optimization

We discuss the case of shape optimization problems with boundary cost functional. We investigate certain theoretical properties and an important tool is the implicit parametrization theorem. Our approach enters fixed domain methods, with known advantages from the implementation point of view. From the geometric point of view, we

allow general perturbations involving both boundary and topological variations.

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CP8

Development of An Effective Collaboration Scheme for Multiple Carriers Based on Data Mining and Meta-Heuristic Optimization Approach

Development of an effective cooperation scheme for multiple carriers is an important issue. The goal of this paper is to develop a cooperation mechanism to endow carriers with the ability to allocate the requests received from customers to cooperative partners flexibly and cost effectively by combining data mining technology with meta-heuristic optimization approach. The data mining technology clusters the requests and allocates them to carriers based on the origins and destinations of requests as well as the location of depots of carriers. A meta-heuristic optimization algorithm is then applied to find delivery routes for carriers to optimize the cost. The simulation results indicate that the performance of the multiple cooperative carriers significantly outperforms that of the multiple non-cooperative carriers. The results of this paper pave the way for the development of an effective collaboration scheme for multiple carriers to gain competitive advantage. This paper is supported in part by the Ministry of Science and Technology, Taiwan, under Grant NSC102-2410-H-324-014-MY3.

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CP8

On the Solution of Operator Equation Problems with Application to Preisach Density Estimation

We study numerical solution of a linear, compact, integral operator equation with linear inequality constraints on the solution space. We present and compare four methods for regularization of the discretized equation without constraints including two new methods. We present two new algorithms solving the linear inequality constrained, minimum norm, least squares problem and compare them with MatLab© function *quadprog*. For high condition numbers, the new methods outperform *quadprog* with lower residual error and solution bias.

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CP8

Globally Convergent Semismooth Newton Methods in Nonsmooth Regularization

We are concerned with Tikhonov regularization of ill-posed problems with nonsmooth penalty functionals. For the computation of the Tikhonov minimizer, we consider a class of B(ouligand)-semismooth Newton methods and discuss their efficient globalization by inexact line search. In numerical tests, our approach proves to be more efficient than other well-established iterative minimization schemes with global convergence. The talk is based on joint work with Esther Hans (University of Mainz)

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CP8

Optimal Transport for Seismic Full Waveform Inversion

Full waveform inversion is a PDE constrained optimization where unknown coefficients in a computed wave field are adjusted to minimize the mismatch with the measured data. We propose using Wasserstein metric based on optimal transport for measuring this mismatch. Several advantageous properties are proved. The Wasserstein metric is computed by solving a Monge-Ampere equation and an algorithm for computing its gradient for the optimization is developed. Finally, numerical examples show quantitative properties.

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CP9

Chaotic Behaviour Of The Shift Map On The Generalized Symbol Space And Topological Conjugacy

This paper aims to study chaotic behavior of the shift map s on the generalized symbol space ?m, m an integer. We prove that s is Devaney chaotic , as exact Devaney chaotic, mixing Devaney Chaotic, Auslander Yorkes chaotic and generically d-chaotic. Also it is established that ?m is a Cantor set and the shift map s on ?m is topologically conjugate to the mod-map on the unit circle S1.

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CP9

Instability in Payoff Positive Game Dynamics

Cressman has shown that a smooth payoff positive game dynamic has a linearization that is a non-negative constant times the linearization for the replicator dynamics. We will use this to show that, in a game of Rock-Paper-Scissors where the payoff associated with losing is larger in absolute value than the payoff associated with winning that no payoff positive game dynamic with nontrivial linearization can be asymptotically stable at the unique Nash equilib-

rium. This result will be extended to include all continuous payoff positive game dynamics using other methods.

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CP9

Modeling the Segregation of a Herd of Cows by Assessing Hunger, Fatigue and Risk

Activity synchronization of animal groups to assure spatial coherence encounters low efficiency. The efficiency can be maximized by segregating a group into subgroups such that the activities are homogeneous within subgroups. Thus, we model the beneficial segregation of a herd of cows using a cost function quantifying their variation of hunger, variation of fatigue and risk from predators. The cost function is minimized over all plausible subgroups those can be created from a known herd.

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CP9

Network-Theoretic Analyses of Vortex Dynamics

Unsteady fluid flows have complex dynamics due to the nonlinear interactions amongst vortical elements. We use network-theoretic tools to characterize vortical interactions to gain insights into the behavior of vortical flows. Dense fluid flow graphs, with vortices as nodes and induced velocity as edge weights, can be distilled to the key structure using spectral sparsification, while preserving nonlinear dynamics and invariants. We further characterize 2D turbulence as a weighted scale-free network and evaluate its resilience.

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CP9

Fractional Dynamics with Distributed Age Initial Condition

The Fractional Fokker-Planck equation has been highly successful in modeling subdiffusion, a process whose mean squared displacement grows slower than linearly in time. Its big drawback, however, is that the initial condition implicitly assumes that at $t = 0$, all particles are motile. Based on the Semi-Markov property of fractional diffusion, we present a physical model and a numerical scheme which can incorporate an initial condition that relaxes this assumption.

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CP10

Ultra-High-Dimensional Optimization Approach to Requirements Development for Acquisition Programs

Requirements for defense acquisition programs have traditionally been developed somewhat in isolation with limited regard for interactive effects, too often resulting in program cancellation and billions of dollars spent with little tangible return. This research seeks to improve defense acquisition by enabling a deep understanding of the interactions and potential conflicts between system requirements during their inception and suggesting defensible, mutually compatible goals that satisfy multiple stakeholders through an ultra-high-dimensional optimization approach.

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CP10

Reference-Based Almost Stochastic Dominance Rules with Application in Risk-Averse Optimization

Stochastic dominance is the preference relation of uncertain prospect defined over a given class of utility functions. While this utility class represents basic properties of risk aversion, it includes some extreme utility functions rarely characterizing a rational decision maker' preference. In this paper we introduce reference-based almost stochastic dominance (RSD) rules which well balance the general representation of risk aversion and the individualization of a decision maker's risk preference. The key idea is that, in the general utility class, we construct a neighborhood of the decision maker's individual utility function, and represent a preference relation over this neighborhood. The RSD rules reveal the maximum dominance level quantifying the decision maker's robust preference between alternative choices. We also propose RSD constrained optimization model and develop an approximation algorithm based on Bernstein polynomials. The model is illustrated on a portfolio optimization problem.

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CP10

Optimization of Integrated Energy Supply Systems by Minlp

We consider an optimization problem of municipal energy supply systems. Under the background of growing penetration of decentralized generation technologies, our goal is to design cost-efficient and *integrated* supply systems of electricity and heat. We propose a mixed-integer nonlinear programming model to solve the problem. Due to the high

complexity of the problem, it is challenging to compute optimal solutions. We apply approximation techniques and exploit specific problem structures to improve solutions for real-world applications.

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CP10

Computationally Expensive Optimization Problems with Hidden Constraints

Optimization problems with computationally expensive black-box objective functions arise in many application areas where the function evaluation requires running a simulation. Surrogate model algorithms have been widely used as solution approach. Difficulties in applying surrogate model algorithms emerge when simulation model runs fail (for example, the underlying solver does not converge) and no objective function value is obtained (hidden constraints). We introduce a surrogate model algorithm that is able to deal with this challenge.

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CP10

A Duality Approach For Sparse Representation In Classification

We apply the selective nature of sparse representation studying a dual formulation of the problem and exploiting the properties of a convex optimization model. Preliminary results with applications in the areas of supervised learning, feature selection and dictionary learning for reduced-order models are presented under this framework.

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CP10

Epigraphical Convergence of Sample Averages of a Random Lower Semi-Continuous Functional Generated by a Markov Chain

The main result in this article is to establish epigraphical convergence of the sample averages of a random lower semi-continuous functional to its expectation, when the sample is a Harris recurrent Markov chain with stationary distribution π. That result is then used to provide a convergent method to solve a stochastic optimization problem involving an expectation functional of the form $E_\pi[f(x,\xi)]$. Moreover, we develop asymptotic normality of optimal solutions and optimal values using Markov chain central limit theorem.

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CP11

Lateral Trait Transfer Enhances Cooperation

In many biologically relevant scenarios, traits may pass laterally between individuals (e.g. in horizontal gene transfer or social behavior imitation), blind to any direct fitness effects that the trait may bestow upon the individuals reproductive fitness. Using game theoretic analyses, we show how incorporating blind imitation into evolutionary dynamics can dramatically enhance the prevalence and stability of cooperative behaviors in social dilemmas. This effect is qualitatively insensitive to the exact details of underlying birth-death-imitation dynamics.

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CP11

Functional Segmentation of Marketing Technologies via Topological Methods

The marketing technology ecosystem is gargantuan, consisting of a rapidly fluctuating set of thousands of vendors shifting in response to market demands and computational resources. Each technology has a distinct browser spectroscopic signature, sequentially requesting and receiving data resources of varying types and quantities. We have developed a highly scalable autonomous process for collecting functional signatures from millions of web domains and identifying functionally similar technologies with topological and information theoretic methods.

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CP11

Forecasting Chaotic Business Cycles Perturbed by Noise

The failure of the Federal Reserve to timely raise its target short-term interest rate to a normal rate of 3.5% skews economic forecasts, causing uncertainty in the economy. By applying a Sprott nonlinear dynamical system, it becomes possible to forecast chaotic business cycles. When interest rates are normal, the economy mean-reverts, like a Langevin equation, perturbed by noise. Then business cycles no longer exist.

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CP11

The Carrying Capacity Allocation Model for Express Freight and General Cargo Under the Price Elasticity of Demand

The time-definite express freight delivery common carriers publish tariffs and deliver express freight shipments door-to-door with guaranteed delivery times. The carriers also bid the time-indefinite general cargo to fill up otherwise unused carrying capacity. The carrying capacity allocation model is to determine prices for express freight and also to decide whether to bid the general cargo so as to fill the available carrying capacity in a way that maximizes profit. We modeled this integral-constrained concave program in link formulation and demonstrated computationally using Taiwans largest time-definite LTL freight carrier.

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CP11

Control Chart for Simultaneous Monitoring of Linear Profile Parameters

Nowadays, Linear profiles are more common because of their simplicity and coverage of more common scenarios. The term profiling is used for association among study and predictor variable(s). In this study, we have designed and investigated EWMA-3 chart under the different ranked set sampling strategies such as ranked set sampling, median ranked set sampling, extreme ranked set sampling and their modifications. The computational results of ARL revealed that the ranked set based EWMA-3 chart offer better detection ability.

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CP11

Users Dynamics on Two-Sided Platforms

I will discuss a dynamic model of two-sided platform, which estimates the volume of users interacting through the platform. I formulate and prove theorems describing the long-term behavior and tendency of this dynamical system. First, I consider generic attachment functions, and obtain a concrete result, formulated in terms of properties of attachment functions. This result is followed by examples, of some two-sided market scenarios, showing how adjustments of attachment functions can influence the users' dynamics. The dynamical systems approach allows natural generalization to multi-sided platform.

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CP11

Do Prices Coordinate Markets?

Walrasian equilibrium prices can be said to coordinate markets because they support a welfare optimal allocation in which each buyer is buying their most preferred goods. However, prices alone are not sufficient to coordinate the market, and buyers may need to coordinate to find a feasible allocation. We provide a genericity condition such that for buyers with Matroid Based Valuations, overdemand with respect to equilibrium prices is at most 1, even with uncoordinated tie-breaking.

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CP12

On the Influence of Surface Chemistry and Vibration on Sedimentation of Pigments in Liquid Coating Formulations

Liquid coating formulations such as latex paints may form irreversible sediments during storage or transportation, causing significant economic losses to manufacturers or end-users. We develop a two phase mathematical model which takes into consideration the surface chemistry at the fluid-particle interface and vibration of the container to elucidate the sedimentation and consolidation process. Our computer simulations indicate that formulating a slightly flocculated dispersion could significantly improve product shelf life.

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CP12

Conservative DEC Discretization of Incompressible Navier-Stokes Equations on General Surface Simplicial Meshes

A conservative discretization of incompressible Navier-Stokes equations over surfaces is developed using discrete exterior calculus (DEC). The current discretization employs barycentric dual meshes, instead of circumcentric duals used in previous DEC-based discretizations. While DEC-based schemes that use circumcentric duality require Delaunay triangulations to work properly, the current scheme admits general surface simplicial meshes, simplifying the task of surface mesh creation. The discretization scheme is presented along with numerical tests demonstrating numerical convergence and conservation properties.

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CP12

Coupled RapidCell and Lattice Boltzmann Models to Simulate Hydrodynamics of Bacterial Transport in Response to Chemoattractant Gradients in Confined Domains

The RapidCell model was developed to simulate E. coli chemotaxis with spatiotemporally varying chemoattractant gradients, which is suited for motility simulations in unbounded non-fluid environments. This limits its use in biomedical applications hinging on bacteria-fluid dynamics in microchannels. We couple the RapidCell model with the colloidal lattice-Boltzmann model to simulate trajectories of self-propelled chemotactic particles in initially stagnant fluids in bounded domains. The chemotactic particles reached the chemoattractant source with the success rates of 20-72%.

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CP12

A Dynamical System for Interacting Flapping Swimmers

We present the results of a theoretical investigation into the dynamics of interacting flapping swimmers. Our study is motivated by recent experiments using a one-dimensional array of wings that swim within each others wakes in a water tank. We develop and analyze a discrete dynamical system in which the swimmers are modeled as airfoils that shed point vortices. Our model may be used to understand how schooling behavior is generally influenced by hydrodynamics.

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CP12

Analysis of High-Speed Rotating Flow in 2D Polar $(r-\theta)$ Coordinate

The generalized analytical model for the radial boundary layer in a high-speed rotating cylinder is formulated for studying the gas flow field due to insertion of mass, momentum and energy into the rotating cylinder in the polar $(r-\theta)$ plane. The analytical solution includes the sixth order differential equation for the radial boundary layer at the cylindrical curved surface in terms of master potential (chi), which is derived from the equations of motion in a polar $(r-\theta)$ plane. The linearization approximation (Wood & Morton (JFM-1980); Pradhan & Kumaran (JFM-2011); Kumaran & Pradhan (JFM-2014)) is used, where the equations of motion are truncated at linear order in the velocity and pressure disturbances to the base flow, which is a solid-body rotation. Additional assumptions in the analytical model include constant temperature in the base state (isothermal condition), and high Reynolds number, but there is no limitation on the stratification parameter. In this limit, the gas flow is restricted to a boundary layer of thickness $(Re^{-1/3}R)$ at the wall of the cylinder. Here, the stratification parameter $A = \sqrt{((mO^2R^2)/(2k_BT))}$. This parameter A is the ratio of the peripheral speed, OR, to the most probable molecular speed, $\sqrt{(}2k_BT/m)$, the Reynolds number $Re = (\rho_w \Omega R^2/mu)$, where m is the molecular mass, and Omega and R are the rotational speed and radius of the cylinder, k_B is the Boltzmann constant, T is the gas temperature, ρ_w is the gas density at wall, and mu is the gas viscosity. An important finding is that the stagnation pressure (no mass flow through the intake tube) is significantly affected by the wall gap, as well as with stratification parameter, indicating a strong coupling between the local temperature, density, pressure and velocity fields.

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CP12

Stretching a Filament for a Viscoelastic Constitutive Model with Thixotropic Yield Stress Behavior

The transient behavior of stretching a filament governed by a viscoelastic constitutive model that combines a Partially Extending strand Convection model with a Newtonian solvent is studied. The filament is fixed at the bottom and the top is pulled up and held. An axisymmetric circular slender jet approximation is used. Gravity and surface tension are included, though they are not the primary mechanisms in this study. Thixotropy and yield stress are possible consequences of our assumption that the ratio of retardation time to relaxation time is a small parameter. An asymptotic analysis leads to a criterion for immediate yielding versus delayed yielding.

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CP12

On Solutions of the 2D Navier-Stokes Equations with Constant Energy and Enstrophy

It is not yet known if the global attractor of the space-periodic 2D Navier-Stokes equations contains nonstationary solutions $u(x,t)$ such that their energy and enstrophy per unit mass are constant for every $t \in (-8,8)$. The study of the properties of such solutions was initiated in [6], where, because of the hypothetical existence of such solutions, they were called ghost solutions. In this work, we introduce and study geometric structures shared by all ghost solutions. This study leads us to consider a subclass of ghost solutions for which those geometric structures have a supplementary stability property. In particular, we show that the wave vectors of the active modes of this subclass of ghost solutions must satisfy certain supplementary constraints. We also discover a computational way to check for the existence of these ghost solutions. (This is a joint work with B.S. Zhang)

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CP13

A Cellular Automaton Model Examining the Effects of Oxygen, Hydrogen Ions and Lactate on Early Tumour Growth

Some tumours are known to exhibit an extracellular pH that is more acidic than the intracellular, creating a 'reversed pH gradient' across the cell membrane and this has been shown to affect their invasive and metastatic potential. Tumour hypoxia also plays an important role in tumour development and has been directly linked to both tumour morphology and aggressiveness. In this paper, we present a hybrid mathematical model of intracellular pH regulation that examines the effect of oxygen and pH on tumour growth and morphology. In particular, we investigate the impact of pH regulatory mechanisms on the cellular pH gradient and tumour morphology. Analysis of the model shows that: low activity of the Na^+/H^+ exchanger or a high rate of anaerobic glycolysis can give rise to a "fingering" tumour morphology; and a high activity of the lactate/H^+ symporter can result in a reversed transmembrane pH gradient across a large portion of the tumour mass. Also, the reversed pH gradient is spatially heterogeneous within the tumour, with a normal pH gradient observed within an intermediate growth layer, that is the layer between the proliferative inner and outermost layer of the tumour.

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CP13

Robust Optimization of Gas Assisted Gravity Drainage Process under Geological Uncertainties

This research purpose is to determine an actual optimal solution through optimization of gas-injection in oilfields. 100 stochastic reservoir realizations were created honoring geological constraints. Ranking was applied to select P10,P20,,P90 that represent the reservoir uncertainty. More than 400 training simulation runs were created through Latin Hypercube Design to build the proxy model, which then verified by 200 extra-runs. The uncertainty was quantified to provide degrees of freedom for decision-makers to reduce the project risk.

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CP13

Algorithms and Analysis for Nonequilibrium Langevin Dynamics

The project is interested in methods to sample particle systems that have an overall steady, homogeneous flow. One application of this dynamics is to impose a strain rate on a complex fluid or immersed molecular system in order to compute the stress-strain constitutive relation using a microscopic stress formulation. We also discuss algorithmic aspects of nonequilibrium molecular dynamics simulations. In such a simulation the simulation box deforms with the flow, and we describe particular boundary conditions that allow for long-time simulation by avoiding extreme deformation of the unit cell.

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CP13

Filters of the Improvement of Multiscale Data from Atomistic Simulations

In multiscale models combining continuum approximations with first-principles based atomistic representations, the dominant computational cost is typically the atomistic component of the model. In this talk we demonstrate the effectiveness of a spectral filter for improving the accuracy of noisy data obtained from atomistic simulations. We show that filtering enables us to run less expensive atomistic simulations to reach the same overall level of accuracy, thereby lowering the primary cost of the multiscale model and leading to faster simulations. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-681476

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CP13

The Effect of a Variable Viscous Profile on the Stability of Multi-Layer Radial Porous Media and Hele-Shaw Flows

In this talk, we will discuss viscous fingering instabilities of multi-layer immiscible Hele-Shaw flows in a radial flow geometry. In particular, we will consider the potentially stabilizing effect of having fluids with a variable viscous profile as part of the displacement process. This problem is motivated by such processes in Enhanced Oil Recovery and has the potential to aid in improving recovery techniques. We study the stability through both a linear stability analysis and numerical simulations.

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CP13

New Explicit Analytical Solutions to Boundary-Value Problem for Poissons Equations in Application to Groundwater Hydrology/Geomorphology

Dirikhlets BVP for the PE governs steady-state groundwater flow in a mound formed by infiltration [1]. We present explicit solution for a wedge-shaped domain with equipotential boundary conditions on the wedge sides, resulting in a hyperboloidal mound. The discharge vector components, streamlines, quantity of groundwater seeping through segments of the wedge sides, near-vertex volume of groundwater are evaluated. A mixed BVP is solved for a circular triangle as flow domain for the model of gully evolution [2]. [1]Strack, O. D. L. 1989. Groundwater Mechanics. Prentice-Hall, Inc., Englewood Cliffs, New Jersey. [2]Petroff, A.P. Devauchelle, O., Seybold H., and Rothman, D.H., 2013.Bifurcation dynamics of natural drainage networks. Philosophical Transactions A, Royal Society, 371(2004)DOI: 10.1098/rsta.2012.0365

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CP13

Spatial Adaptivity in Stochastic Simulations

Localized descriptions of random fields, such as Markov random fields, provide a means of coupling spatial and stochastic variations. In this talk, we leverage this feature to develop an algorithm for achieving spatial adaptivity in the stochastic setting, through the use of localized, statistical *a posteriori* error estimators. We illustrate our method by investigating the effect of random surface roughness on the behavior of laminar flow through a pipe.

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CP14

Intermediate Materials Alleviate Stress Concentration at Tissue Interfaces

Material interfaces of vastly different Young's moduli, such as bone-to-ligament, develop a stress concentration when subject to tensile loads. To alleviate this, animals are hypothesized to use a transitional region. We test this hypothesis using a 2D elastic model of a transitional region with graded Young's modulus, derive scaling relationships for dependence of its length on the geometric and elastic properties of the adjoining materials, and compare against biological data.

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CP14

Estimation of Shear Stress in Machining by Inversion of Abel Transform

Despite many years of study, the determination of accurate constitutive response models for the flow stress in materials for finite-element simulations of high-speed machining operations remains a difficult open problem. We present a new approach to the problem of estimating shear flow stress in machining. The recent invention of a cutting tool that is transparent in infrared frequencies makes it possible to obtain good in-situ temperature measurements along the chip-tool interface during a steady-state machining operation. By solving a convection-diffusion problem that models the flux of heat into the chip and the tool during a cutting process, the temperature distribution along the tool face can be shown to satisfy a Volterra integral equation of the first kind with a weakly singular kernel, Abel's equation, for the determination of the flow stress. Because the temperature data are experimentally determined, estimation of the flow stress by inversion of the Abel equation under these circumstances is an ill-posed problem. We discuss current progress in finding an approximate solution of this unstable inverse problem using the Truncated Singular Components Method of Rust. As an application of this method, we give estimates of the flow stress in the work material on the tool face for a series of orthogonal cutting tests on AISI 1045 steel at three different depths of cut.

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CP14

Design Issues for Magnetic Rulers

We deal with the design of a magnetic ruler as an absolute positioning system. Trapezoid-shaped magnetic areas are placed side by side, so that the resulting pattern enables a unique encoding of each position up to a micrometer level. The problem of finding a longest-possible ruler is formulated as a linear mixed-integer problem. We demonstrate how to approximate the magnetic signal, using measured data from Hall sensor cells. From there, we discuss how the absolute position is recovered.

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CP14

Stasis Domains in the Locomotion of a Bio-Inspired Crawler

Thanks to the research on bio-inspired soft robots, the modelling of crawling locomotors is receiving increasing attention. In this talk we see how, in case of dry friction, the locomotion problem for a N-segments crawler can be restated and solved in the framework of rate-independent systems. Hysteresis is described through the introduction of stasis domains and the role of a directionality in the friction is discussed.

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CP14

An Efficient Integral Equation Solver for Two-Dimensional Simulations in Nanoplasmonics

Nanoplasmonics forms a major part of the field of nanophotonics, which explores how electromagnetic fields can be confined over dimensions on the order of or smaller than the wavelength. Here, we present an integral-equation formulation of the mathematical model that delivers accurate solutions in small computational times for surface plasmons coupled by periodic corrugations of at surfaces. Scheme we propose is based on high-order (spectral) treatment of the (integral-equation formulation of the) mathematical models and they deliver highly accurate solutions in significantly lower computational times than the classical existing methods.

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CP14

Boundary Integral Equation Method in the Theory of Thermoelasticity of Double Porosity Materials

The theory of thermoelasticity of double porosity materials has found applications in many branches of civil engineering, geotechnical engineering, technology and biomechanics. In this talk the linear theory of thermoelasticity for materials with a double porosity structure is considered and the boundary value problems (BVPs) of the steady vibrations are investigated. The fundamental solution of system of equations of steady vibrations is constructed. The uniqueness theorems of the internal and external BVPs of steady vibrations are proved. The basic properties of surface (single-layer and double-layer) and volume potentials are established. The existence of regular solution of the BVPs by means of the boundary integral equation method and the theory of singular integral equations are proved.

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CP15

An $O(N)$ Mol$^{\mathbf{T}}$ Energy Gradient Flows Using Direct Operator Inversion for Phase Field Models

We extend the Method of Lines Transpose (MOL$^{\mathrm{T}}$) framework based on successive convolution to phase field models that come from energy gradient flows. The fundamental solver has arbitrary order of accuracy in space, and is based on inversion of a modified Helmholtz equation, with fast $O(N)$ convolution. Higher orders of accuracy in time are then constructed through traditional implicit time stepping methods combined with ideal fixed-point iteration. Numerical simulation results for the 4th and 6th order nonlinear equation in multi-dimensions are provided.

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CP15

Multigrid KSS Methods for Time-Dependent PDE

Krylov Subspace Spectral (KSS) methods are traditionally used to solve time-dependent, variable-coefficient PDEs. Lambers, Cibotarica, and Palchak improved the efficiency of KSS methods by optimizing the computation of high-frequency components. This talk will demonstrate how one can make KSS methods even more efficient by using a multigrid-like approach for low-frequency components. The essential ingredients of multigrid, such as restriction, residual correction, and prolongation, are adapted to the time-dependent case. Numerical experiments demonstrate the effectiveness of this approach.

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CP15

Efficient Time-Stepping Methods for the Numerical Solution of Large Stiff Systems Within Parabolic Partial Differential Equations

The discretization of time-dependent parabolic partial differential equations by a method of lines approach results in a system of stiff ordinary differential equations (ODEs). As a testbed we use a coupled non-linear multi-species advection-diffusion-reaction model in three space dimensions for Calcium Induced Calcium Release in a heart cell. We study Singly Diagonally Implicit Runge-Kutta (SDIRK) and Rosenbrock methods as alternatives to the established backward differentiation formulas.

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CP15

Partition of Unity Isogeometric Analysis of Elliptic Singular Perturbation Problems

The design basis functions on the reference domain in IGA are diversified and enhanced by extra enrichment functions and various local refinements with use of partition of unity function with flat-top. With this method the corresponding stiffness matrix has a small bandwidth and local refinement is simple. Here we apply this method to various boundary layer problems.

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CP15

Adaptive BDDC Methods for Problems Posed in $H(\mathrm{div})$

A BDDC preconditioner consists of a coarse component, expressed in terms of primal constraints and a weighted average across the interface between the subdomains, and local components given in terms of Schur complements of local subproblems. Our BDDC methods are based on an adaptive selection of primal constraints developed to deal with highly oscillating coefficients. Bounds on the condition number of the preconditioned system are also provided which are independent of the values and jumps.

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CP15

Investigation and Numerical Solution of the Difference Analogue of One Nonlinear Parabolic Equation

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

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial x}\left(k\left(x,\, t,\, U\right)\frac{\partial U}{\partial x}\right) + f\left(x, t, U\right)$$

is considered. For the mentioned difference scheme the convergence of its solution to the solution of the source problem is proved when certain conditions hold. For the same difference scheme the comparison theorems and the existence and uniqueness of its solution is proved for the same conditions. The iteration process for finding difference scheme solution is constructed and its convergence is proved.

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CP16

A Compact Scheme on the Cubed Sphere Grid for Propagation Problems in Climatology

In this presentation, we give an account on recent results obtained with a finite difference scheme on the Cubed-Sphere grid [J.-P. Croisille *Hermitian compact interpolation on the Cubed-Sphere grid, Jour. Sci. Comp*, 57,1, 2013, pp.193–212]. High-order accuracy is reached by using a specific compact scheme. Numerical results on advection

test cases of interest in Computational Climatology will be shown [M. Brachet and J.-P. Croisille, *Numerical simulation of vortex propagation problems on the Cubed-Sphere using a compact scheme*, Preprint, 2016]. Test-cases involving the linearized Shallow Water equations will be displayed as well. In addition, results on the mathematical analysis of the scheme will be given.

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CP16

Study of a Model Equation in Detonation Theory: Multidimensional Effects

We extend our work on a reactive Burgers equation in order to include multidimensional effects. Furthermore, we explain how the model can be rationally justified following the ideas of our recently developed asymptotic theory of detonations. The proposed model is a forced version of the unsteady small disturbance transonic flow equations. We show that for physically reasonable choices of forcing functions, traveling wave solutions akin to detonation waves exist. It is also demonstrated that multidimensional effects play an important role in the stability and dynamics of the traveling waves. Numerical simulations indicate that solutions of the model tend to form multi-dimensional patterns analogous to cells in gaseous detonations.

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CP16

Interior and Boundary Spikes for the Two-Dimensional GM System

We prove the existence of assemblies of interior and boundary spikes as stationary solutions of the two-dimensional Gierer-Meinhardt system. Moreover, we also discover that the locations of the spikes are determined by the curvature of the domain boundary together with the Green's function of the domain. A reflection operator of $-\Delta$ is introduced to study the behavior of the regular part of Green's function around the boundary. This reflection generalizes the well-known notions of mirror image and circle inversion for domains with sufficiently smooth boundary.

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CP16

A Numerical Scheme for Two Dimensional Hyperbolic Partial Differential Equations

In this article, a numerical scheme based on finite difference and polynomial differential quadrature method is developed for numerical solutions of two dimensional hyperbolic partial differential equations with initial and Neumann boundary conditions. In the development of the scheme, the first step is semi-discretization in time with forward finite difference and then obtained system is fully discretized by differential quadrature method. Finally, we obtain a Lyapunov system of linear equations which is solved by Matlab solver for the system. Numerical results are obtained for sine-Gordon and Telegraph equations.

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CP16

Global Attractors and Weak Exponential Attractors for Strongly Damped Wave Equations with Nonlinear Hyperbolic Dynamic Boundary Conditions

We discuss the well-posedness and asymptotic behavior of a strongly damped semilinear wave equation equipped with nonlinear hyperbolic dynamic boundary conditions.

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CP16

A Triple Bubble Solution in a Quaternary Inhibitory System

A quaternary inhibitory system motivated by the copolymer theory is studied as a nonlocal geometric variational problem. The free energy of the system is the sum of two terms: the total size of the interfaces separating the four constituents, and a longer ranging interaction energy that inhibits micro-domains from unlimited growth. In a particular parameter range there is a triple bubble solution that exists as a stationary set of the free energy functional. The constructive proof of the existence theorem reveals much information about the solution. The proof also implies a kind of stability.

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CP17

Spectral Geometry of Families of Large Sparse Stieltjes Matrices via Examples

Identification of Stieltjes matrices with resistive electrical networks, yields graph Laplacians and canonically associated zeta-functions. Finite element (FE) discretizations of Dirichlet BVPs lead to Stieltjes matrices and a zeta-functions correspondence associated with the BVP and underlying graph. Consideration of FE discretizations of Laplace-like BVPs under h-refinement as a function of the domains dimension, yields families of zeta-functions of graphs, predictable spectral asymptotics, and a conjectured size-independent characterization of graphs with excluded minors via their zeta-functions.

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CP17

Properties of Linear Multiparameter Matrix Pencils and Applications to Matrix Operator Systems

The study of matrix pencils and matrix operator systems forms a very important focal point in linear algebra. In this paper, we present results on properties of matrix pencils via tensor products of matrices in Hilbert spaces. Lastly, we give generalizations to multi-parameter matrix operator systems and subsystems.

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CP17

Graph Signal Classification Using Wavelet Packet Dictionaries and the Lasso

Lasso methods are well-known in the statistics community for obtaining sparse solutions to classification and regression problems given an overcomplete dictionary of basis vectors. We use Lasso for classifying signals on a graph, and demonstrate the effectiveness and explanatory power of using wavelet packet coefficients formed from hierarchical partitioning of the graph as features. For term-document matrix analysis, we find that this method yields meaningful groups of terms for classifying and characterizing documents.

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CP17

Improved Functionality and Performance for the Spike Banded Solver

The SPIKE algorithm uses a domain decomposition technique to obtain parallelism in the matrix factorization and solve operations for block tridiagonal matrices. One example of such a matrix is the frequently encountered band matrix. We present a new SPIKE based solver for banded matrices, including a newly designed transpose solve operation. With the inclusion of a transpose solve option, SPIKE gains feature-parity with the standard LAPACK solvers, but with significantly improved parallel performance.

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CP17

Computing Geodesic Rotations

An element of a *flag manifold* is a frame—a decomposition of Euclidean space into orthogonal components—and a geodesic path on a flag manifold provides a “direct’ rotation from one frame to another. Furthermore, a geodesic path corresponds to a decomposition of unitary matrices that generalizes the CS decomposition. We develop efficient methods for numerical computation on a flag manifold, including the location of geodesic paths, and consider a question of uniqueness.

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CP18

Destriping of Remote Sensing Imagery by Optimizing An Inverse Problem

Striping is a commonly pronounced artifact in many remote sensing images which occurs mainly due to the variations of calibrations from detector to detector. We present a destriping method by developing a functional to smooth the stripes while preserving the rest. The destriped image may be uncovered by optimizing the functional using a variational method. Also we demonstrate our method on two different striped data sets (VIIRS and HICO).

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CP18

Economical Finite-Difference Scheme for One System of Nonlinear Multi-Dimensional Partial Differ-

ential Equations

Economical finite-difference scheme for one system of nonlinear multi-dimensional partial differential equations is constructed. In particular case model can be used as a mathematical simulation of process of vein formation in meristematic tissues of young leaves. Stability and convergence of developed scheme are proven. Numerical experiments verifying theoretical findings for three-dimensional case are carried out. The appropriate graphical illustrations are given.

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CP18

On the Stability of Stationary Solution and Numerical Approximation for One Nonlinear Model

Nonlinear One-dimensional model based on Maxwell system is considered. Initial-boundary value problem with mixed boundary conditions is studied. Necessary and sufficient condition for linear stability of stationary solution is given. The Hoph-type bifurcation is also observed. Global exponential stabilization of solution is also proved for partial case. The finite difference-scheme is constructed and studied for this case of nonlinearity. Numerical experiments are fulfilled and appropriate results are presented.

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CP18

Full Waveform Inversion for Microseismic Event Estimation

Unconventional oil and gas recovery is of great interest due to the profitability of hydraulically fracturing rock to remove hydrocarbons from low permeability materials such as shale. This injection of water at high pressures, however, may induce tiny microseismic events (earthquakes). These events can be used to illuminate the subsurface in inversion studies. We discuss using full waveform inversion to determine the character of these microseismic events even when the data is noisy and uncertain.

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CP18

Randomization for Efficiently Computing Reduced Order Models in Nonlinear Parametric Inversion

In nonlinear inverse problems, the forward problem typically requires solving many large-scale discretized PDEs. This is often the dominant cost for these problems. Reduced order models are one way to reduce this cost. However, computing the reduced order model still requires solving many systems. We aim to reduce this cost by randomization.

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CP18

On the Upper Bound of the Kolmogorov Entropy of the Weak Global Attractor of the 3D Navier-Stokes Equations

Taking the Kolmogorov ε entropy as a measure of the complexity of the weak global attractor of the 3D Navier-Stokes equations and using the squeezing property of the trajectories of the solutions, we are able to bound the Kolmogorov ε-entropy explicitly in terms of the Grashof number, a physical parameter of the flow.

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CP19

Flow Field Free, Image Processing Inference If Coherence, From Jupiter Observations, With Koopman Operator Connections

Viewing a data set such as clouds of Jupiter, coherence is readily apparent to human observers, such as the Great Red Spot, and other great storms and persistent structures. We describe image processing inference of coherent sets from a fluidic system directly from image data, without attempting to first model underlying flow fields, by a modified kernel kmeans method. We then show connections to a Koopman operator formalism, connecting the method to theoretical considerations.

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CP19

New Phenomena in Dynamic Hopf Bifurcation: Spatial Delays, Spatial Memory Effects, and How Persistent Fluctuations on Nonlinear Ramps Influence the Memory Effect

In dynamic Hopf bifurcation problems the transition to large amplitude oscillations may not occur until a slowly changing parameter is considerably beyond the value predicted from the static bifurcation analysis (delay effect), and the onset may be dependent on the initial value of the slow parameter (memory effect). Here we show **spatial delays** and **spatial memory effects** for a reaction diffusion equation. In addition we show how persistent fluctuations influence delay/memory effects for nonlinear ramps.

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CP19

Identifying the Coupling Structure in Complex Systems Through the Optimal Causation Entropy Principle

Inferring coupling structure of complex systems from time series data is a challenging problem in applied science. The reliability of statistical inferences requires construction of information-theoretic measures taking into account both direct and indirect influences, manifest in as information flows between the components within the system. We present application of the optimal causation entropy (oCSE) principle to identify coupling structure by aggregative discovery for progressive removal algorithms based on the oCSE principle, from measured data.

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CP19

Real and Complex Behavior for Networks of Coupled Logistic Maps

Many natural systems are organized as networks, in which the nodes interact in a time-dependent fashion. For ensemble iterations of maps coupled as nodes in a network, we investigate the relationship between the system's architecture and dynamics, and we discuss possible extensions of the traditional Fatou-Julia theory for single map iterations. We illustrate how the system's asymptotic behavior in both the real and complex case (measured via topological properties of the Julia sets) changes when perturbing the underlying adjacency graph. We differentiate between the effects on dynamics of different operations that directly modulate network connectivity: (1) increasing/decreasing edge weights, (2) increasing/decreasing edge density, (3) altering edge configuration by adding, deleting or moving edges.

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CP19

Inference of Boolean Networks Using Optimal Causation Entropy

Boolean dynamics is widely used in the modeling of biological systems, in particular cellular network dynamics. An important problem in practice regards how to accurately infer a Boolean network from observational data, especially when the underlying system consists of a large number of units. Using the recently developed theory of optimal causation entropy, we devised an efficient computational approach to infer Boolean networks from data, and demonstrate its utility using both synthetic and experimental examples.

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CP19

Autoresonance and Mathieu Stability Boundaries

Driving a Duffing nonlinear oscillator at its low-amplitude oscillation frequency does not sustain resonant amplitude growth. Amplitude-frequency dependence results in an amplitude and frequency modulated beat. Sweeping the drive frequency sustains resonance and is called autoresonance.
Mathieu stability analysis provides a novel means of investigating autoresonance stability in Duffing oscillators. It is found that autoresonance onset maps to the primary Mathieu resonance stability boundary, evolving to a stable region as amplitude growth rate diminishes.

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CP20

GPU-Accelerated Bernstein-Bezier Dg Methods for Wave Problems

The computationally intensive nature of time-explicit nodal discontinuous Galerkin (DG) methods is well-suited to implementation on Graphics Processing Units (GPUs). We evaluate Bernstein-Bezier bases as an alternative to nodal polynomials for DG discretizations and show how to exploit properties of derivative and lift operators specific to Bernstein polynomials. Efficiency and numerical stability are discussed in the context of a model wave propagation problem, and computational experiments comparing the two bases are presented.

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CP20

Density Estimation for a Class of Elliptic Problems on Stochastically Perturbed Domains

We study elliptic PDEs for which the domain is uncertain. Of particular interest is the nonparametric density estimation problem for a quantity-of-interest. We introduce a piecewise transformation of the domain to a deterministic reference domain and exploit this in a Monte Carlo sampling procedure to approximate the distribution efficiently. We present an a-posteriori error analysis for the empirical distribution function obtained from the samples, which reflect the various deterministic and statistical sources of error.

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CP20

Analysis of the Parallel Schwarz Method for the Solution of Chains of Particles in the Solvation Model

A new class of Schwarz methods was recently presented in the literature for the solution of solvation models, where the electrostatic energy contribution to the solvation energy can be computed by solving a system of elliptic partial differential equations [1] and related references. Numerical simulations have shown an unusual convergence behaviour of Schwarz methods for the solution of this problem, where each particle corresponds to a subdomain: the convergence of the Schwarz methods is independent of the number of particles [1], even though there is no coarse grid correction. Despite the successful implementation of Schwarz methods for this solvation model, a rigorous analysis for this unusual convergence behaviour is required, since no theoretical results are given in the corresponding literature. In this talk, we analyze the behaviour of the Schwarz method for the solution of a chain of particles and show that its convergence does not depend on the number of particles. We use three different techniques to prove this result: the first technique is based on a Fourier expansion of the error and on the analysis of transfer matrices, the second consists in an application of the maximum-principle and the third is a variational approach that allows us to regard the Schwarz method as an alternating projection method. [1] Cancès et al., Domain decomposition for implicit solvation models, J. of Chem. P. (2013).

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CP20

Asynchronous Optimized Schwarz Methods for the Solution of Pdes

Asynchronous methods are parallel iterative procedures where each process performs its task without waiting for other processes to be completed. For the numerical solution of a general PDE on a domain, Schwarz iterative methods use a decomposition into two or more (overlapping) subdomains. In the classical formulation, Dirichlet boundary conditions are used on the artificial interfaces. Given an initial approximation, the method progresses by solving the PDE in each subdomain using as boundary data on the artificial interfaces the values of the solution on the neighboring subdomain from the previous step. This procedure is inherently parallel. For optimized Schwarz, the boundary conditions on the artificial interfaces are of Robin or mixed type. Thus, one can optimize the Robin parameter(s) obtaining a very fast method. We present an asynchronous version of the optimized Schwarz method for the solution of differential equations on a parallel computational environment. In a one-way subdivision of the computational domain, with overlap, the method is shown to converge when the optimal artificial interface conditions are used. Convergence is also proved under very mild conditions on the size of the subdomains, when approximate (non-optimal) interface conditions are utilized. Numerical results are presented on large three-dimensional problems illustrating the efficiency of the proposed asynchronous parallel implementation of the method.

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CP20

Overcoming Order Loss in High Order Runge-Kutta Methods for Initial Boundary Value Problems

This work focuses on a fundamental problem that arises with high-order time-stepping in initial boundary values problems: a loss of convergence order incurred with Runge-Kutta methods. We describe the underlying mechanism that leads to order loss via numerical analysis, and provide

a remedy that is based on modifying the boundary conditions. Numerical tests show that this approach recovers full convergence order of the time-stepping schemes.

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CP21

On Two-Dimensional Nonlinear Integro-Differential Equation Associated with the Penetration of a Magnetic Field into a Substance

One two-dimensional nonlinear partial integro-differential equation is considered. The model arises in mathematical simulation of electromagnetic field penetration into a substance electro-conductivity of which essentially depends on temperature. Initial-boundary value problem with Dirichlet homogeneous boundary conditions is considered. Large time behavior of solution is studied. Rate of stabilization is given. Various numerical experiments are carried out. Results of numerical experiments with the corresponding graphical illustrations are given.

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CP21

Lie Symmetry Analysis and Dust-Acoustic Waves in Dusty Plasma Modeled by Burgers Type Equation

In this work, the Dust-acoustic waves in dusty plasma modeled by nonlinear Burgers' type equation are studied through Lie symmetry approach. Using suitable similarity transformations, the given Burgers' type equation is reduced to ordinary differential equations (ODEs). During the procedure of reduction, sometime we got some highly nonlinear ODEs which are not easily solvable for traveling wave solutions. Therefore, numerical methods are applied to the reduced ODEs for constructing Dust-acoustic waves.

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CP21

Haar Wavelet Based Method for Numerical Simulation of Parabolic Burgers' Equation with Variable Coefficients

In this work we analyze the viscous Burgers' equation with variable coefficients which arises in fluid and plasmas. Numerical simulation of Burgers' equation using Haar wavelet is necessary as its exact solution is not available in literature. Variety of numerical techniques based on FDM and FEM etc are fails due to some disadvantages such as; poor continuity, global support, poor spatial localization. To get overcome from these disadvantages we have proposed Haar wavelet method which is compactly supported and orthogonal. Using Haar wavelet collocation method Burgers' equation leads to a system of linear algebraic equations which are solvable.

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CP21

Evolutionary Singularly Perturbed Problems and Their Efficient Numerical Simulations

In this talk, I will discuss some complexities involved with simulation of evolutionary singularly perturbed problems. Then I will present construction and analysis of a robust numerical method that is applicable to solve this class of problems. Non-trivial but relevant extensions to solve systems of such partial differential equations will also be addressed. Finally, some simulation results along with the application of the proposed approach in other fields will be presented.

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CP21

On the Existence and the Asymptotic Stability of Solutions to the Rotating Boussinesq Equations for the Atmosphere and Ocean

The author studies the rotating Boussinesq equations describing the motion of a viscous incompressible stratified fluid in a rotating system which is relevant, e.g., a Lagrangian and Eulerian analysis of a geophysical fluid flow. These equations consist of the Navier-Stokes equations with buoyancy-term and Coriolis-term in beta-plane approximation, the divergence-constraint, and a diffusion-type equation for the density variation. They are considered in a plane layer with periodic boundary conditions in the horizontal directions and stress-free conditions at the bottom and the top of the layer. Additionally, the author considers this model with Reynolds stress, which adds hyper-diffusivity terms of order 6 to the equations. This manuscript focuses primarily on deriving the rotating Boussinesq equations for geophysical fluid dynamics, showing existence and uniqueness of solutions, and outlining how Lyapunov functions can be used to assess energy stability. The author also addresses singular problems for which the equation has parabolic structure (Rotating Boussinesq equations for the atmosphere and ocean) and the singular limit is hyperbolic (Quasi-Geostrophic equations for the atmosphere and ocean) in the asymptotic limit

of small Rossby number. In particular, this approach gives as a corollary a constructive proof of the well-posedness of the problem of quasi-qeostrophic potential vorticity equations governing modons or Rossby solitons.

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CP22

A Global-Local Optimization Template for Multiple History-Matched Reservoir Parameters

Parameterization of petroleum reservoirs is an important component of reservoir management. However, the process of reservoir parameterization is fraught with nonuniqueness. Nonuniqueness leads to large uncertainty and risks in reservoir management. One way to reduce and quantify the uncertainty in parameter estimation is to generate multiple realizations of the parameters. We introduce an algorithm that generates multiple realizations of reservoir parameters by performing global optimization at a coarse-scale and local optimization at a finer scale.

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CP22

Fast Minimum Uncertainty Estimates for the Exponential Fitting Problem

With vast amounts of data, exponential fitting is expensive due to inner-products in the Gauss-Newton method. By projecting measurements onto a particular subspace, we replace an $O(n)$ operation inner-product with an $O(1)$ closed-form sum formula. This drastically reduces operation count and, with proper subspace choice, yields high precision parameter estimates. For example, projecting a $n = 10^5$ magnetic resonance spectroscopy problem onto a 400-dimensional subspace yields estimates 98% as accurate and 100× faster than the original.

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CP22

Uncertainties in Coherent X-Ray Diffractive Imaging 3D Reconstructions

Modern coherent X-ray technology provides possibilities to acquire huge amounts of single-biomolecules diffraction patterns. These two-dimensional patterns can be reconstructed to a few ngstrms resolution. However, this task is developing and highly resolved reconstructions have not been produced. We analyze the current best-in-practice algorithm by isolating the different sources of uncertainties. Our main contribution is a methodology in the form of bootstrap for critical assessing uncertainties, which will be critical when handling large data.

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CP22

Accelerating Newton's Method for Semilinear Parabolic Control Via Reduced-Order Modeling

We use reduced order models (ROMs) to substantially decrease the computational cost of Newtons method for semilinear parabolic optimal control problems. Rather than generating a reduced order model to replace the original problem, we use the structure of Hessian and subspace-based ROMs to compute approximate reduced order Hessian information. The resulting method is convergent. Numerically it often enjoys convergence rates similar to those of Newtons method, but at the computational cost of the gradient method.

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CP22

Proper Symplectic Decomposition for Forced and Dissipative Hamiltonian Systems

Many DDDAS applications rely on reduced order models to speed up the calculations. Recently, the proper symplectic decomposition (PSD) is proposed to model reduction for large-scale Hamiltonian systems while preserving the symplectic structure [SIAM J. Sci. Comput., 38 (2016), pp. A1A27]. In this talk, we reformulate dAlemberts principle to Hamiltonian form, and extended PSD for model reduction of forced and dissipative Hamiltonian systems. As an empirical approach, PSD preserves dissipativity and stability, thus, PSD is better suited than the classical POD for model reduction of hyperbolic PDEs.

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CP22

Approximation of Dynamical Systems with Nonlinear Frequency Dependence via a Structure-preserving Model Reduction Algorithm

Large-scale dynamical systems pose significant computational difficulties when used in numerical simulation. Model reduction is one response to this challenge. We consider here dynamical systems with a nonlinear frequency dependence, for which we cannot obtain a standard first-order realization. Such systems may have realizations that reflect important structural features of the model and we may wish to retain this structure in the reduced model. We present a structure-preserving model reduction algorithm for such systems.

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CP22

Automatic Dimensionality Reduction Using Gaussian Processes: Application to High Dimensional Uncertainty Quantification

We develop a gradient-free approach to dimensionality reduction using active subspaces, which is robust to observational noise. We rely on Gaussian process regression to develop our surrogate model and represent the active subspace as an orthogonal projection matrix, which serves as a hyperparameter of the Gaussian process model. We use recent results on orthogonality-constrained optimization to compute maximum likelihood estimates for the hyperparameters and demonstrate the application of this novel approach to three numerical examples.

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CP23

A Multigene Genetic Programming for Thyroid Disorder

Two diseases of thyroid gland, which releases hormones for regulating metabolism, are hyperthyroidism and hypothyroidism. Before patients are classified as being normal or suffering from hyperthyroidism or hypothyroidism, tests are conducted by existing models which are costly. We present the detection of thyroid disorder based on Multigene Symbolic Regression Genetic Programming technique. The results show the model is good and is able to reduce attributes classifying patients as Normal, Hyperthyroidism and Hypothyroidism.

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CP23

Genetic Toggle Switch in the Absence of Cooperative Binding

We present an analytical treatment of a genetic switch model consisting of two mutually inhibiting genes operating without cooperative binding of the corresponding transcription factors. Previous studies have numerically shown that these systems can exhibit bimodal dynamics without possessing two stable fixed points at the deterministic level. We analytically show that bimodality is induced by the noise and find the critical repression strength that controls a transition between the bimodal and nonbimodal regimes. We also identify characteristic polynomial scaling laws of the mean switching time between bimodal states. These results, independent of the model under study, reveal essential differences between these systems and systems with cooperative binding, where there is no critical threshold for bimodality and the mean switching time scales exponentially with the system size.

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CP23

A General Framework for the Analysis of Infectious Disease Models with Delayed Differential Equations

Most mathematical models for infectious disease follow the compartmental framework implemented by Kermack and McKendrick in the early 1900s. Since then, mathematical epidemiology has expanded this technique to include many different disease dynamics – notably incubation periods, seasonality, and treatment. More recently, van den Driessche and Watmough showed how to calculate the basic reproduction number ($\mathcal{R}_0$) of such models. Here, we expand this framework to include biological phenomenon that may be modeled using delay differential equations.

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CP23

Mathematical Model of Ischemia-Reperfusion Injury and Postconditioning in a Two-Dimensional Channel

Reperfusion (restoration of blood flow) after a period of ischemia (interruption of blood flow) can paradoxically place tissues at risk of further injury: so-called Ischemia-Reperfusion Injury or IR injury. Recent studies have shown that postconditioning (intermittent periods of further ischemia applied during reperfusion) can reduce IR injury. We develop a mathematical model to describe the reperfusion and postconditioning process following an ischemic insult, treating the blood vessel as a two-dimensional channel, lined with a monolayer of endothelial cells that interact (respiration and mechanotransduction) with the blood flow. We investigate how postconditioning affects the total cell density within the endothelial layer, by varying the frequency of the pulsatile flow and the oxygen fluctuation at the inflow boundary. We find that, in the scenarios we consider, the high pulsatile flow reduces cellular damage and constant influx of O_2 or low frequency fluctuations of O_2 at the inflow boundary increases the rate of cell proliferation.

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CP23

Minimal Sensor Networks for Detecting Non-Diffusive Disease Spreading

Disease outbreaks and epidemics may propagate non-diffusively due in part to the heterogeneity of human contact networks. Given finite resources to detect epidemics constrained by these complex, dynamic topologies, we investigate optimal sensor placement strategies. We model spatial transmission of diseases on various types of networks using continuous-time random walks with power law step-size and waiting-time distributions for infected individuals. We adapt principles of compressive sensing to optimize sensor coverage and include effects of intrinsic and extrinsic noise.

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CP23

Modelling of the Ebola Disease: The Most Deadly Disease of Our Time?

The recent outbreak of Ebola disease blossomed into a full pandemic in some countries in west africa. This disease is highly infectious between individuals. Symptoms include fever, severe headache,muscle pain, weakness, fatigue, diarrhea, vomiting, abdominal pain and unexplained hemorrhade. This presentation is aimed at using mathematical modeling technique to describe the spread of Ebola disease in Guinea, liberia, Sierraleon and Nigeria, to understand the effect of quarantine in the control of Ebola virus disease, to make prediction about the future trend of the disease. The novelty in this project is addition of dead and quarantine class in the dynamics of the disease spread.

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CP24

Eigenfunction Expansions for Legendre's Equation

We revisit Legendre's equation

$$-\big((1-x^2)y'(x)\big)' + \left(\frac{1}{4} + \frac{\ell^2}{1-x^2}\right) y(x) = \lambda y(x), \qquad (2)$$

and investigate the eigenfunction expansions on $(-1,+1)$ for $\ell \in [0,\infty)$. Our m-functions are normalized with respect to suitably normalized Frobenius solutions. This novel approach gives rise to interesting new results and, for $\ell \geq 1$, requires the Krein-Langer theory of Generalized Nevanlinna Functions. See also: Fulton and Langer, Sturm-Liouville Operators with Singularities and Generalized Nevanlinna Functions, Complex Anal. Oper. Theory (2010) 4, 179-243.

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CP24

New Preconditioned Exponential Time Integrators for Stiff Differential Equations

We propose two new classes of time integrators for stiff DEs: the implicit-explicit exponential (IMEXP) and the hybrid exponential methods. In contrast to the existing exponential schemes, the new methods offer significant computational advantages when used with preconditioners. Any preconditioner can be used with any of these new schemes. This leads to a broader applicability of exponential methods. The proof of stability and convergence of these integrators and numerical demonstration of their efficiency are presented.

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CP24

Stiffness Detection Metrics for Chemical Kinetics

This study investigates stiffness quantification metrics capable of efficiently and robustly determining the appropriate category of integrator required for chemical kinetics. Stiffness quantification methods are surveyed and used to investigate chemical kinetics states, including methods based on eigendecomposition or the spectral radius of the Jacobian matrix, error estimations, conditioning parameters, and computational cost estimations. These methods are applied to hydrogen and methane autoignition, and evaluated in terms of effectiveness and computational efficiency.

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CP24

Improving the Efficiency of Stiffly Accurate Exponential Propagation Iterative Methods of Runge-Kutta Type (epirk)

In a recent paper we extended the theory developed for exponential Rosenbrock methods [Hochbruck,Ostermann,Schweitzer,Vu] to construct stiffly accurate EPIRK schemes. These new methods are guaranteed to converge with an expected order given that the underlying problem satisfies certain regularity conditions. For classically derived methods the flexibility of the EPIRK framework allowed derivation of particularly efficient schemes that take advantage of the adaptive Krylov method. However, the same approach does not work for stiffly accurate EPIRK schemes due to restrictions imposed by the stiff order conditions. We propose a new method of constructing and implementing the stiffly accurate EPIRK integrators that allows us to achieve efficiency comparable to and competitive with the classical schemes. We present a set of numerical experiments that illustrate the performance of these new time integrators.

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CP24

Mathematical Model and Numerical Simulations of the Transmission Dynamics of Ebola Virus

Ebola hemorrhagic fever is a highly infectious and lethal disease. The recent Ebola epidemic outbreak in West Africa is the most complex outbreak since the virus was first discovered in 1976. In this paper a mathematical model for the transmission dynamics of Ebola virus among humans is presented. The model assumes that no one leaves or enters the susceptible human population immediately the disease starts. The formulated model is a system of ordinary differential equations and is analyzed employing the theories of dynamical system. The analysis of the steady state and its stability show that the system will be stable if there is a bound on contacts among the humans within the study population. We also explored the sensitivity of the final epidemic size to the starting time of intervention and results show that the rapid implementation of contact measures should be considered a critical component in any contingency plan against Ebola disease outbreaks for which no specific treatment exists.

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CP25

High Efficiency Sixth Order Computation with Richardson Extrapolation for Elliptic PDEs

By using Richardson extrapolation on two fourth order approximate solutions from different scale grids, a sixth order numerical solution can be computed on the coarse grid. Then, other techniques can be applied to obtain a sixth order numerical solution on the fine grid. No extra cost is needed to build such kind of grids if multigrid methods are involved as the solver for the resulting linear system.

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CP25

A High-Order Scheme for the Biharmonic and the Navier-Stokes Equations in Irregular Domains

We propose a high-order compact method for the approximation of the biharmonic and Navier-Stokes equations in planar irregular geometry. This is based on a fourth order Cartesian Embedded scheme for the biharmonic problem [M. Ben-Artzi, I. Chorev, J-P. Croisille and D. Fishelov "A compact difference scheme for the biharmonic equation in planar irregular domains", SIAM J. Numer. Anal., 47, 2009, pp.3087–3108.] where a bidimensional Lagrange-Hermite polynomial was introduced. A variety of numerical results asses fourth-order convergence rates. In addition, a purely one dimensional procedure was designed for the Navier-Stokes equations. Numerical results demonstrate fourth-order convergence rates.

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CP25

Partitioned Methods for Contaminant Transport Models in Coupled Groundwater-Surface Water Flows

Partitioned methods uncouple models for surface-water with groundwater flows into subdomain, subphysics solves. The resulting (Stokes-Darcy) fluid velocity is important because the flow transports contaminants. The numerical analysis and algorithm development for the evolutionary Stokes-Darcy-transport problem has, focused on a quasi-static Stokes-Darcy model and a single domain (fully coupled) formulation of the transport equation. In this research, however, we examine the computational and numerical difficulties of the fully evolutionary system, in which a nonlinear term in the convection-diffusion equation arises from the nonzero divergence of the velocity in the porous media domain. The nonlinear term acts as a reaction term, coupling the growth rate to the error in the discrete convecting velocity. This imposes regularity restrictions on the convecting velocity to ensure stability. We present a numerical analysis of a partitioned method for contaminant transport for the fully evolutionary system. The algorithm studied and presented is unconditionally stable and requires only one subdomain solve per step.

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CP25

High-Order Absorbing Boundary Conditions for Discontinuous Galerkin Time-Domain Schemes

Discontinuous Galerkin finite element schemes exhibit attractive features for large-scale wave-propagation simulations on modern parallel architectures. In order to limit the size of the computational domain, these schemes must be coupled with nonreflective boundary conditions, which remains a challenging task. In this talk, we present a coupling of high-order absorbing boundary conditions with nodal discontinuous Galerkin schemes. Numerical results are proposed to validate both the accuracy and the computational efficiency of the techniques.

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CP25

Numerical Study of a Dielectric Barrier Discharge Phenomena and Its Effect on the Air Flow

We present a numerical method we developed in order to simulate the effect of the dielectric barrier discharge actuators on the air flow. Hence, we compute the potential and electric field distribution, respectively, and the electron and the ion density and velocity evolution in a prescribed setting. Afterwards we compute the air velocity field influenced by those entities. The method is demonstrated on a set of numerical tests in three-dimensional domain inspired by real-life experiments.

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CP26

Wetting and Dewetting of Thin Viscoelastic Drops

We present a numerical study of thin viscoelastic drops on solid substrates, and study the dynamics of spreading and receding subject to van der Waals interactions. We consider Jeffreys model for viscoelastic stresses and investigate the effects of viscoelasticity on wetting and dewetting dynamics. Elastic effects are found to lead to deviations from Cox-Voinov law for partially wetting Newtonian fluids. We show that viscoelasticity enhances spreading and suppresses retraction, compared to Newtonian drops.

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CP26

An Interpolative Particle Level Set Method

Capturing topological changes for multiphase flow problems remains a challenge. The front running approaches are level set methods and Lagranian particle methods, but both have their drawbacks. Hybrid particle-level set hybrid methods can alleviate these problems. Our approach uses particles adjacent to the level set to get a smooth and accurate interface with minimal additional particles. We are able to accomplish this by using an interpolation scheme to update grid points near the interface using the distances of nearby particles and increase the accuracy of the level set approach without limiting it to the refinement of the grid size. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

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CP26

Multi-Scale Modeling of Compaction-Initiated Detonation in Heterogeneous Explosives

In heterogeneous explosives, sites of high temperature and pressure, called hot spots, play a significant role in detonation initiation. This study seeks to model hot spots generated by the compaction of a granular explosive. Two scales are considered, a macro scale modeled as compressible reactive flow with compaction coupled to a grain scale represented by a reaction-diffusion system. Well-resolved numerical results are presented for detonation initiation as well as for steady-state detonation.

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CP26

Optimum Permeability Profile and Fouling in Membrane Filters

A reasonable question that membrane filter manufacturers may ask is: what is the optimal configuration of filter membranes, in terms of internal morphology (pore size and shape), to achieve the most efficient filtration? In order to answer this question, we must first propose a robust measure of filtration performance. Filter membrane performance can be measured in a number of different ways. As filtration occurs the membrane becomes blocked, or fouled, by the impurities in the feed solution, and any performance measure must take account of this. For example, one performance measure might be the total throughput – the amount of filtered feed solution – at the end of filtration process, when the membrane is so badly blocked that it is deemed no longer functional. Here we present a simplified mathematical model, which (i) characterizes membrane internal pore structure via pore or permeability profiles in the depth of the membrane; (ii) accounts for various membrane fouling mechanisms (adsorption, blocking and cake formation); and (iii) defines a measure of filter performance; and (iv) predicts the optimum pore or permeability profile for our chosen performance measure.

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CP26

Simulating Surfactant Spreading: Impact of a Physically Motivated Equation of State

A single model for the spreading of surfactant-driven thin liquid films has dominated previous literature. However, discrepancies exist between this model and experimental results in the surfactant spatial distribution and the spreading timescale. Here, we present numerical simulations that demonstrate the impact of the equation of state relating the surfactant concentration to the surface tension and propose an empirically-motivated equation of state which resolves some discrepancies and raises new issues to be pursued in experiments.

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CP26

An Efficient Particle Vortex Method for Vorticity Dynamics in Free Space

We present an efficient particle vortex method for directly simulating the fluid flow motion in free space. The method employs techniques to accelerate the computation (adaptive mesh refinement and MPI parallelism) and maintain the accuracy and stability of the solutions (vorticity remeshing, high order interpolation). For the case of inviscid flow, a comparison to the inviscid elliptic dipole computation is made to validate the method. For the viscous case, some preliminary results will be presented.

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CP26

A VMS-FEM for Monolithic ALE Computations of Shock Hydrodynamics

We present a stabilized FEM for monolithic arbitrary Lagrangian-Eulerian (ALE) shock hydrodynamics. It differs from the commonly used Lagrangian/remap strategy, and provides additional flexibility of handling inflow/outflow boundary conditions. The method extends a variational multiscale (VMS) stabilization for Lagrangian flows to ALE ones, and employs the entropy viscosity to capture shocks. We present extensive examples to demonstrate the robustness and versatility of the method, and end the talk with its application to multiphase flow computations.

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CP27

High Throughput Chemical Toxicity Screening As a Bayesian Signaling Game

Catching chemicals that may be toxic to humans or the environment early in production is critical to saving costs. We will demonstrate how to use Adverse Outcome Pathways and high throughput chemical screening data in a Bayesian signaling game context to efficiently make go/no-go screening decisions and design test batteries for chemical hazard screening. The views and opinions expressed are those of the individual authors and not those of the U.S. Army.

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CP27

Optical Biosensors for Multicomponent Reactions

Optical biosensors determine rate constants by measuring only the mass change on a reacting surface in real time. Hence it can be difficult to analyze data from multiple simultaneous reactions. We reduce a set of coupled PDEs in the experimental surface-volume geometry to a set of coupled integrodifferential equations using asymptotics. The reduced model is solved numerically and analytically for typical multicomponent reactions. Experimental protocols are given that will allow the analysis of individual reactions given lumped data.

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CP27

A Mathematical Model to Elucidate Brain Tumor Abrogation by Immunotherapy with T11 Target Structure

T11 Target structure (T11TS), a membrane glycoprotein isolated from sheep erythrocytes, reverses the immune suppressed state of brain tumor induced animals by boosting the functional status of the immune cells. This study aims at aiding in the design of more efficacious brain tumor therapies with T11 target structure. We develop a mathematical model for malignant gliomas or brain tumor and the immune system interactions, by introducing the role of immunotherapeutic agent/drug T11TS. The model encompasses considerations of the interactive dynamics of malignant glioma cells, macrophages, cytotoxic T- lymphocytes (activated CD8+ T - cells), immune-suppressive factor TGF-β, immune-stimulatory factor IFN-γ and the T11TS. We performed sensitivity analysis in order to determine which of the state variables are more sensitive to the given system parameters. The results of the proposed mathematical model are compared with experimental data procured by our collaborator Prof. Dr. Swapna Chaudhuri, Immunology Lab, Department of Hematology, School of Tropical Medicine, Kolkata, India. Computer simulations were used for model verification and validation, which underscore the importance of T11 target structure in brain tumor therapy.

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CP27

Optimal Mating Strategies for Preferentially Outcrossing Simultaneous Hermaphrodites in the Presence of Predators

We develop an optimization model to understand the life-history evolution of preferentially outcrossing simultaneous hermaphrodites in the presence of predators. When mates are unavailable, sexually mature individuals may reallocate resources towards defense and/or future reproduction instead of selfing. We determine the optimal delay before selfing under a variety of conditions including differing strategies of predators and strength of inbreeding depression. The results are compared with recent experiments on *Physa acuta*, a species of freshwater snail.

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CP27

Mathematical Modeling of Nanocarrier Distribution in the Microvasculature

Nanomedicine is a new drug-delivering system that use nanoparticles for selective targeting in the tumor regions. For understanding nanoparticle transport in the microvasculature, it is helpful to use mathematical and computational models. In this talk, a mathematical model of nanoparticle distribution in the microvasculature is introduced to capture the underlying physics in nanomedicine design. For achieving this goal, nanoparticle movements in blood flow are predicted by coupling several mathematical models. Then, the nanoparticle transport model is combined with in silico microvasculature. The entire system is tested for predicting nanoparticle accumulation in the normal and tumor microvasculature. The simulation results and future perspectives will be fully discussed.

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CP27

Scaling and Similarity of Biological Joints

Joints in the limbs of animals are either flexures or ligaments. Flexures are absent in animals that are larger than a few millimeters. Scaling and stability considerations show that biological flexures are severely limited in their range of rotation, to ~ 0.2 radians, independent of size. Such movement-limited joints cannot support external loads, and distal adhesive pads become necessary to exert external forces. Flexures are therefore limited to

millimeter-scale animals where adhesion is effective.

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CP28

Formulation of a Discontinuous Galerkin Method for Unstructured Causal Grids in Spacetime and Linear Dispersive Electromagnetic Media

We present a spacetime discontinuous Galerkin formulation for time domain (TD) electromagnetics problem with local and asynchronous solution features. Using differential forms, we formulate the problem for arbitrary domains in spacetime and linear dispersive media. A novel recursive method is proposed to derive the auxiliary differential equations required for the analysis of dispersive media in TD. We present the methods energy stability proof, solutions for some TD benchmark problems, and convergence rate numerical verifications.

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CP28

From Discrete Time Random Walks to Numerical Methods for Fractional Order Differential Equations

We present a numerical method, based on a stochastic process, for solving a class of fractional partial differential equations. The scheme is derived from the master equations for the evolution of the probability density of the process. The diffusion limit of the master equations guarantees the consistency of the numerical scheme and stability results are simply obtained. This highlights the broader applicability of using discrete stochastic processes to provide numerical schemes for fractional differential equations.

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CP28

An Arbitrary Order, Fully Implicit, Hybrid Kinetic Solver for Radiative Transport Using Integral Deferred Correction

An implicit, hybrid method for linear kinetic equations was recently proposed and an implementation using the implicit Euler method was studied. We present an arbitrarily high order solver based on this hybrid method using integral deferred corrections with respect to the implicit Euler method. Several convergence studies and multiple test problems are provided to show the efficacy of the hybrid method extends to implicit methods of higher order in both highly collisional and non-collisional regimes.

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CP28

A Non-Stiff Method for Airy Flow: Application to the Modified Korteweg De Vries Equation.

We adapt the non-stiff, interface tracking methods developed by Hou-Lowengrub-Shelley to the modeling of 2-D curves whose motion obeys Airy flow, a dispersive, nonlinear and curvature dependent geometric evolution law. Strikingly the curvature evolves according to modified Korteweg de Vries equation. Particularly, we present a non-stiff numerical scheme, a fully discrete space-time proof of convergence, linear analysis and numerical evidence that confirms accuracy, convergence and stability of the method.

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CP28

Multigrid Methods for Systems Arising from High Order CVFEM Discretizations

On modern computing architectures, high order discretizations are appealing due to smaller mesh requirements, better accuracy, and high numerical intensity. A question is whether linear systems arising from such discretizations can be solved via multigrid, the method of choice for first order discretizations of elliptic PDEs. We consider multigrid applied to high order CVFEM discretizations arising from low Mach fluid flow problems. We discuss appropriate smoother choices and coarsening strategies, and conclude with numerical results.

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CP28

Construction and Analysis of a Weighted Sequential Splitting Method for the 3D Maxwell's Equa-

tions

We present a Weighted Sequential Splitting (WSS) finite difference time-domain method for Maxwell's equations in three dimensions. The construction and analysis of the WSS method, main results as well as numerical experiments are given that illustrate and confirm our theoretical results.

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CP29

Lyapunov-Based Robust Reduced Order Model Stabilization for Partial Differential Equations: Application to the Coupled Burgers Equation

The problem of reducing a partial differential equation (PDE) model to a system of finite dimensional ordinary differential equations (ODE), is of paramount importance in engineering and physics where solving such PDE models is too time consuming. The idea of being able to reduce the PDE model to a simple model, without loosing the main characteristics of the original model, such as stability and prediction precision, is appealing for any real-time model-based computations. However, this problem remains challenging, since model reduction can introduce stability loss and prediction degradation. To remedy these problems, many methods have been developed aiming at what is known as stable model reduction. In this paper, we focus on the so-called *closure models* and their application in reduced order model (ROM) stabilization. We present results on robust stabilization for reduced order models (ROM) of partial differential equations using Lyapunov theory. Stabilization is achieved via closure models for ROMs, where we use Lyapunov theory to design a new closure model, which is robust with respect to model structured uncertainties. Furthermore, we use a learning algorithm to optimally tune the closure models' parameters, for optimal ROM stabilization. The coupled Burgers' equation is employed as a test-bed for the proposed stabilization method.

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CP29

Stochastic Partial Functional Differential Equations with Delay

We will present our recent results on the existence and uniqueness of strong solutions to stochastic partial functional differential equations (SPFDEs) with locally monotone coefficients, locally Lipschitz nonlinearity, and time delay. We note that, while SPFDEs have important applications, they are far less studied than SPDEs and SFDEs. Our results extend and widen the applicability of those of Liu-Röcker (2010), Caraballo et al (2000), and Taniguchi et al (2002). We illustrate the applicability of our results by applying them to a stochastic 2D Navier-Stokes equation with time delay, and a stochastic Nicholson's blowflies equation with time delay.

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CP29

Fundamental Gaps and Energy Asymptotics of the Gross-Pitaevskii/nonlinear Schrodinger Equation with Repulsive Interaction

We study asymptotically and numerically fundamental gaps (i.e. difference between the first excited state and the ground state) in energy and chemical potential of some specially defined Gross-Pitaevskii equations (GPE) with repulsive interaction under box potential or harmonic potential. And some gap conjectures will be formulated based on our results. Finally, we'll extend our results to the GPE on bounded domains with either the homogeneous Neumann boundary condition or periodic boundary condition.

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CP29

Interpolation of Functions with Parameter Dependent Jumps by Transformed Snapshots

The prevalence of shocks causes major difficulties for the efficient simulation of parametric and stochastic hyperbolic PDEs. As a remedy, I propose a new interpolation type method that uses additional transformations of the physical domain to align jumps in parameter. The strategy is akin to neural networks, where a function valued interpolation, comparable to stochastic collocation methods, serves as outer layer and transformations of the physical domain as hidden layers.

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CP29

Gepup: Reformulating the Incompressible Navier-Stokes Equations (inse) for Fourth Or Higher-Order Numerical Solutions

Via a commutator of Laplacian and generic projections [Zhang 2015 JSC], we reformulate INSE as the evolution of the projected velocity. Then finite-volume discretization and implicit-explicit time integration lead to extreme accuracy and efficiency: to achieve 3 digits of accuracy of vorticity for a turbulent boundary layer, it is faster to run the proposed method on a personal desktop than to run two classic second-order projection methods on the fastest

supercomputer in the world!

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MS1

Photonic Graphene and Properties

The lecture will begin with a background discussion of nonlinear optical waves which the speaker has been associated with. Then photonic lattices with a honeycomb/hexagonal background, sometimes called ‘Photonic Graphene, will be introduced. Photonic Graphene exhibits novel phenomena. In unbounded lattices the dispersion surfaces touch at Dirac points; this is connected with conical, elliptical and straight-line diffraction. When helically varying waveguides are introduced, traveling edge waves have been experimentally observed. Analysis describing this phenomena shows that traveling linear and nonlinear edge states exist and the envelope of the edge wave satisfies a nonlinear Schrodinger (NLS) equation. The edge mode can be transmitted or reflected across the sharp boundaries and in certain cases have properties that have been associated with topological insulators. NLS solitons also inherit these topological properties previously found for linear waves. Photonic Graphene provides new mechanisms to control light.

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MS1

On the Homogenization of a Transmission Problem in Scattering Theory for Highly Oscillating Periodic Media

We discuss the homogenization of a transmission problem arising in the scattering theory for bounded inhomogeneities with periodic coefficients modeled by the anisotropic Helmholtz equation. The coefficients are assumed to be periodic functions of the fast variable, specified over the unit cell with small characteristic size. By way of multiple scales expansion, we establish higher-order bulk and boundary corrections of the leading-order homogenized transmission problem. The analysis in particular provides rigorous estimates of the error committed by the first-order-corrected solution considering both boundary and bulk correction. We also present explicit boundary corrections for the transmission problem when the scatterer is a unit square and its limit as the cell size goes to zero. At the end we briefly consider the homogenization of the corresponding transmission eigenvalue problem and show that the transmission eigenvalues, which can be determined from the scattering data, can be used to reconstruct the effective material properties of the highly oscillating periodic media. This is joint work with B. Guzina and S. Moskow.

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MS1

Reconstructing Optical and Acoustic Properties in PAT/TAT from Multiple Illumination Data

We consider the problem of simultaneous reconstruction of acoustic and optical properties in quantitative photoacoustic (PAT) and thermoacoustic (TAT) imaging. We will first describe a one-step strategy for the numerical solution of the inverse problem, and then provide some theoretical justifications, including uniqueness and stability of the reconstructions, in simplified settings. We will also present a recent result that characterizes the limitation of the imaging depth in PAT.

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MS1

Title Not Available at Time of Publication

Abstract Not Available at Time of Publication

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MS2

Monolithic Multigrid for Incompressible, Resistive Magnetohydrodynamics

Magnetohydrodynamics (MHD) models describe a wide range of plasma physics applications, from thermonuclear fusion in tokamak reactors to astrophysical models. These models are characterized by a nonlinear system of partial differential equations in which the flow of the fluid strongly couples to the evolution of electromagnetic fields. As a result, the discrete linearized systems that arise in the numerical solution of these equations are generally difficult to solve, and require effective preconditioners to be developed. This talk investigates monolithic multigrid preconditioners for a one-fluid, viscoresistive MHD model in two dimensions that utilizes a second Lagrange multiplier added to Faradays law to enforce the divergence-free constraint on the magnetic field. We consider the extension of a well-known relaxation scheme from the fluid dynamics literature, Vanka relaxation, to this formulation. To isolate the relaxation scheme from the rest of the multigrid method, we utilize structured grids, geometric interpolation operators, Galerkin coarse grid operators, and inf-sup stable elements for both constraints in the system. Numerical results are shown for the Hartmann flow problem, a standard test problem in MHD.

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MS2

High Order Finite Difference WENO Scheme for Ideal Magnetohydrodynamics on Curvilinear Meshes

In this talk, we will present a high-order weighted non-oscillatory (WENO) finite difference constrained transport scheme for ideal magnetohydrodynamic (MHD) equations on curvilinear meshes. The proposed method maintains a divergence-free magnetic field, allows treatment of complex geometries with relative ease, and is capable of resolving complex features with fewer grid points than uniform meshes. Numerical results demonstrate the flexibility, robustness, and high resolution of the proposed method.

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MS2

Locally Implicit Discontinuous Galerkin Methods with Application to the Vlasov-Maxwell System

The Vlasov-Maxwell equations model the dynamics of plasma; in particular, in this work we model laser-plasma interactions and the acceleration of electrons or ions to relativistic energies. These equations contain a large spectrum of temporal and spatial scales, which makes accurate and efficient numerical simulations difficult to obtain. We develop an efficient solver for this system by defining the Regionally Implicit Discontinuous Galerkin Methods, an expansion of the so called Locally Implicit Discontinuous Galerkin method (LIDG) developed in [J. Qiu, M. Dumbser, and C.-W. Shu., Comp. Meth. Appl. Mech. Eng., 194(42-44):45284543, 2005.]. We show that these methods allow a much larger CFL number when compared to the LIDG method.

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MS2

Solving Fluid and Continuum Kinetic Equations in Plasma Physics Using the Discontinuous Galerkin Method

The discontinuous Galerkin method has been used to solve equations in plasma physics in fluid and kinetic regimes. Some challenges in modeling plasmas include the need to resolve disparate scales with physically-relevant dispersive and diffusive phenomena. Additionally, the high-dimensionality of the Vlasov equations has made continuum kinetic simulations inaccessible until recently. Results will be presented using multi-fluid plasma models and direct discretization of the Vlasov-Poisson equation using the discontinuous Galerkin method.

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MS3

Global Convergence Rate of Proximal Incremental Aggregated Gradient Methods

We propose the proximal incremental aggregated gradient (PIAG) method for minimizing the sum of a large number of smooth component functions fi(x) and a convex function r(x). Such composite optimization problems arise in a number of machine learning applications including regularized regression problems and constrained distributed optimization problems over sensor networks. Our method computes an approximate gradient for the function f(x) by aggregating the component gradients evaluated at outdated iterates over a finite window K and uses a proximal operator with respect to the regularization function r(x) at the intermediate iterate obtained by moving along the approximate gradient. Under the assumptions that f(x) is strongly convex and each fi(x) is smooth with Lipschitz gradients, we show the first linear convergence rate result for the PIAG method and provide explicit convergence rate estimates that highlight the dependence on the condition number of the problem and the size of the window K over which outdated component gradients are evaluated.

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MS3

Stochastic Variance Reduction for Nonconvex Optimization

We study nonconvex finite-sum problems and analyze stochastic variance reduced gradient (SVRG) methods for them. SVRG and related methods have recently surged into prominence for convex optimization given their edge over stochastic gradient descent (SGD); but their theoretical analysis almost exclusively assumes convexity. In contrast, we prove non-asymptotic rates of convergence (to stationary points) of SVRG for nonconvex optimization, and show that it is provably faster than SGD and gradient descent. We also analyze a subclass of nonconvex problems on which SVRG attains linear convergence to the global optimum. We extend our analysis to mini-batch variants of SVRG, showing (theoretical) linear speedup due to mini-batching in parallel settings. Joint work with Ahmed Hefny (CMU) , Suvrit Sra (MIT) , Barnabas Poczos (CMU) , Alex Smola (CMU).

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MS3

First-order Methods for Geodesically Convex Optimization

Geodesic convexity generalizes the notion of (vector space) convexity to nonlinear metric spaces. But unlike convex optimization, geodesically convex (g-convex) optimization is much less developed. In this paper we contribute to the understanding of g-convex optimization by developing iteration complexity analysis for several first-order algorithms on Hadamard manifolds. Specifically, we prove upper bounds for the global complexity of deterministic and stochastic (sub)gradient methods for optimizing smooth and nonsmooth g-convex functions, both with and without strong g-convexity. Our analysis also reveals how the manifold geometry, especially *sectional curvature*, impacts convergence rates. To the best of our knowledge, our work is the first to provide global complexity analysis for first-order algorithms for general g-convex optimization. Based on joint work with: Hongyi Zhang (MIT).

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MS3

A Variational Perspective on Accelerated Methods in Optimization

Accelerated gradient methods play a central role in optimization, achieving optimal rates in many settings. While many generalizations and extensions of Nesterov's original acceleration method have been proposed, it is not yet clear what is the natural scope of the acceleration concept. In this work, we study accelerated methods from a continuous-time perspective. We show that there is a Lagrangian functional that we call the Bregman Lagrangian which generates a large class of accelerated methods in continuous time, including (but not limited to) accelerated gradient descent, its non-Euclidean extension, and accelerated higher-order gradient methods. We show that the continuous-time limit of all of these methods correspond to traveling the same curve in spacetime at different speeds. From this perspective, Nesterov's technique and many of its generalizations can be viewed as a systematic way to go from the continuous-time curves generated by the Bregman Lagrangian to a family of discrete-time accelerated algorithms. Based on joint work with Ashia Wilson (UC Berkeley) and Michael Jordan (UC Berkeley)

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MS4

Combinatorial Properties of Hierarchical Models

Associated to a simplicial complex $\mathcal{C}$ with ground set $\{1, 2, \ldots, m\}$ and an integer vector $\mathbf{d} \in \mathbb{N}^m$ is the design matrix $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ for a log-linear model. We are interested in developing techniques for determining when $\mathcal{A}_{\mathcal{C},\mathbf{d}}$ satisfies various "niceness' properties. The case where $\mathbf{d} = \mathbf{2}$, the vector of all 2s, is of particular interest. New results include a complete classification of the simplicial complexes that give rise to unimodular $\mathcal{A}_{\mathcal{C},\mathbf{2}}$, and progress towards the classification problem for compressed and normal $\mathcal{A}_{\mathcal{C},\mathbf{2}}$.

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MS4

Algebraic Regression

Regression is one of the oldest and most well-known methods in statistics. In this talk we'll describe an algebraic generalization of the classic regression paradigm that breaks with the tradition of an explicit functional relationship between predictors and response by instead assuming an implicit representation: that the predictors and response are related by a variety. Many consequent aspects of the model are considered, including parameter and interval estimation, model selection, and an implementation in R.

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MS4

Conditional Independence Ideals with Hidden Variables

Conditional independence (CI) constraints among a collection of discrete random variables can be formulated algebraically in terms of the determinants of certain submatrices of the probability tensor. This allows to associate a corresponding CI variety with each collection of CI statements, and implications among CI statements can be analyzed by studying this variety which contains all probability distributions satisfying the CI constraints. We study the decomposition of this variety into irreducible subsets with a good statistical interpretation, and the irreducible components will be interpreted in matroid terms.

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MS4

Skeletal Structure in the Enumeration of Markov Equivalence Classes

The classic result of Verma and Pearl tells us that two directed acyclic graphs are Markov equivalent if and only if they share the same skeleton and the same set of immoralities. Falling in step with the combinatorial enumeration of other graphical structures such as matchings and independent sets, we investigate the problem of enumerating Markov equivalence classes for a fixed type of skeleton. We also investigate how the skeletal structure can impact the possible sizes of the Markov equivalence classes.

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MS5

Flow Induced by Bacterial Carpets and Transport of Microscale Loads

Experimental work has suggested that the flagella of bacteria may be used as motors in microfluidic devices by creating a bacterial carpet. Mathematical modeling can be used to investigate this idea and to quantify flow induced by bacterial carpets. We simulate flow induced by bacterial carpets using the method of regularized Stokeslets, and also examine the transport of vesicles of finite size by arrays of rotating flagella.

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MS5

Diabetes Susceptibility and Sleep: Modeling Glucose Metabolism under Circadian Disruption

Long-term disruptions to the sleep-wake cycle can alter glucose metabolism and increase susceptibility to type 2 diabetes. Circadian misalignment occurs when the sleep-wake pattern is antiphase with the primary circadian clock. We develop a mathematical model of the glucose-insulin regulatory system with meal absorption to explain experimental data from a clinically forced, progressive circadian misalignment study. The resulting model incorporates circadian dependence of model parameters. Simulation results and long-term metabolic implications are discussed.

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MS5

Modeling the Diffusion of Prion Aggregates in Budding Yeast

Prions are misfolded proteins that self-propagate by converging native proteins to the misfolded form, which are then prone to aggregation. These misfolded proteins are believed to act as the infectious agent in neurodegenerative diseases such as mad cow disease, scrapie, and Creutzfeldt-Jakob disease. The mechanism of prion transmission during cell division is not yet understood. Using data obtained from experiments we have developed a hindered diffusion model for prion aggregate transmission in budding yeast.

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MS5

Synchronization of Tubular Pressure Oscillations by Vascular and Hemodynamic Coupling in Interacting Nephrons

The kidney plays an essential role in regulating the blood pressure and a number of its functions operate at the functional unit of the kidney, the nephron. To understand the impacts of internephron coupling on the overall nephrons' dynamics, we develop a mathematical model of a tubuloglomerular feedback (TGF) system, a negative feedback mechanism for nephron's fluid capacity. Specifically, each model nephron represents a rigid thick ascending limb only and is assumed to interact with nearby nephrons through vascular and hemodynamic coupling along the preglomerular vasculature. We conduct a bifurcation analysis by deriving a characteristic equation obtained via a linearization of the model equations. (Joint work with Anita T. Layton)

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MS6

The Most Current List of Participating Companies Is Available at http://www.siam.org/meetings/an16/career.php

For Career Fair Attendees The career fair will feature representatives from nonacademic employers from industry and government. These representatives will be prepared to discuss with you the opportunities for internships, postdoctoral appointments and full-time jobs at their organizations.

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MS7

Filtering Large-Scale Dynamical Systems Using Transport Maps

Abstract Not Available at Time of Publication

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MS7

Data-Driven Methods for Nonintrusive Model Reduction

The construction of projection-based reduced models typically requires matrix-vector products with the operators of the full model; however, these intrusive matrix-vector products are impracticable if the full model is given as a black box. We present data-driven model reduction techniques that learn the reduced models in a nonintrusive way directly from snapshot data. We demonstrate our data-driven methods on linear models and models with low-order nonlinear terms.

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MS7

Density Estimation Framework for Model Error Quantification

The importance of model error assessment during physical model calibration is widely recognized. We highlight the challenges arising in conventional statistical methods accounting for model error, and develop a density estimation framework to quantify and propagate uncertainties due to model errors in presence of sparse and noisy data. The reformulated calibration problem is then tackled with Bayesian techniques. We demonstrate the key strengths of the method on synthetic cases and on a few practical applications.

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MS7

A Model Reduction Approach to Structural Health Monitoring

We present a Data-Based Approach to the problem of Structural Health Monitoring with synthetic training. The approach exploits (i) synthetic results obtained by solving a PDE model for many values of the parameters, and (ii) machine-learning algorithms to generate a classifier that monitors the systems damage state. Our formulation integrates the reduced-order PDE model within the classification framework and allows to take into account model error. We illustrate our method through a companion micro-truss experiment.

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MS8

Developing a PGAS Graph Library using GraphBLAS Primitives

Partitioned Global Address Sparse (PGAS) languages offer a convenient way to express distributed memory parallelism. The GraphBLAS effort aims to standardize matrix-based primitives for graph computations. In this presentation, we share our experiences of implementing GraphBLAS primitives in PGAS languages. We evaluate expressibility, performance, and composability.

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MS8

GraphBLAS Template Library (GBTL): Implementing Graph BLAS on GPU

GraphBLAS is a set of graph algorithms primitives meant to standardize and unify a set of building blocks for a graph algorithms implementer. We will present our implementation of GraphBLAS primitives implemented in a generic C++ GraphBLAS Template Library (GBTL) library. We will discuss the design of our interface and implementation, and we will discuss preliminary performance results.

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MS8

The Graph Programming Interface and Its Evolution Towards GraphBLAS

We started the development of the Graph Programming Interface (GPI) at IBM Research in 2014, with the goal of providing a common interface for application development and system optimization. Our implementation evolved to leverage the multiple levels of parallelism (processor, cores, threads) and large memory capacity of the IBM POWER8 processor, thus delivering the high performance that Big Data graph analytic applications require. We soon realized that it made sense to participate in the development of a standard for graph computation in the language of linear algebra, as advanced by GraphBLAS, so that a larger ecosystem could develop around it.

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MS8

Design Considerations for a GraphBLAS Compliant Graph Library on Clusters of GPUs

We implement a promising GraphBLAS compliant graph processing library on clusters of GPUs. We examine the scalability of our approach to solving this problem, and the unique challenges posed by the GPU architecture: creating enough computation in communication-bound algorithms, and balancing inter-GPU communication with data replication. We will present results in graph algorithms such as breadth-first search (BFS), single-source shortest path (SSSP), and PageRank.

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MS9

Hierarchical and Multigrid Solvers

Hierarchical solvers are based on leveraging the hierarchical structure of matrices to reduce computational cost and memory footprint. We will show how these methods are related to algebraic multigrid and multilevel solvers. In this context, we will present a numerical analysis of hierarchical solvers, will discuss their convergence, and how the choice of low-rank basis affects the condition number of the preconditioned linear system.

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MS9

STRUMPACK: Preconditioning Using Incomplete Factorization with Hierarchically Semi-Separable Matrices

We present STRUMPACK, a linear solver and preconditioner based on multifrontal LU factorization, developed at LBNL with a BSD license. Dense fill-in in the factors is approximated by hierarchically semi-separable matrices. Low-rank approximations are constructed using randomized sampling. This leads to an efficient preconditioner for many PDE based problems. We present numerical results, comparing our code with state-of-the-art preconditioners like algebraic multigrid and ILU on large parallel machines

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MS9

A Superfast Multi-Rank Eigenvalue Update: Algorithm, Analysis, and Applications

We present some recent developments to the algorithms, analysis, and applications of divide-and-conquer eigenvalue algorithms for hierarchically structured matrices. Our contributions include a novel new approach for the rank-k update to the symmetric eigenvalue problem which is stable, has O(kn log n) complexity, and great data locality. This leads to an elegant approach for dealing with the pathological case of clustered eigenvalues. We test our new algorithms on applications including semidefinite programming optimization problems.

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MS9

Butterfly Factorization for a Class of Transforms in Harmonic Analysis

This talk introduces new techniques of the butterfly factorization for efficient implementation of several transforms in harmonic analysis, e.g., Fourier integral operators (e.g., pseudo differential operators, the generalized Radon transform, the non-uniform Fourier transform, etc.) and special function transforms (including the Fourier-Bessel transform, the spherical harmonic transform, etc.). These techniques lead to nearly optimal operation and memory complexity for constructing and applying the butterfly factorization. They also enable good scalability for high performance computation.

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MS10

Parallel Iterative Solvers for Hybridized DG Methods with Application to Large-Eddy Simulation

We present a mixed-precision Newton-GMRES solver with application to Large-Eddy Simulation (LES). First, we propose a Minimal Residual algorithm to compute a good initial guess for the Newton iteration. We then introduce a Minimum Interaction Domain Decomposition method of general applicability to implicit solvers, and apply it to construct a restrictive additive Schwarz parallel preconditioner. Also, a block incomplete LU (BILU) factorization and a Minimum Discarded Fill reorder algorithm for hybridized DG methods are employed for the subdomain preconditioner. We finally discuss the effect of the stabilization tensor on the BILU factorization and propose some convenient choices to improve the quality of the subdomain preconditioner. The proposed approach will be illustrated through its application to LES of turbulent flows.

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MS10

The HDG Methods for Diffusion Problems

We present an HDG formulation for a model Possion's equation on a polygonal/polyhedral mesh. We then discuss two approaches to devise HDG methods with optimal convergence (or superconvergence) property. The first approach is to systematically modify (or augment) the approximation spaces in a suitable way such that the projection based error analysis [Mathematics of Computation 79 (271), 1351-1367] can be applied. (It is the continuation of the work started [Mathematics of Computation 79 (271), 1351-1367] on searching for "superconvergent" HDG methods). The second approach is to suitably choose the stabilization function (or the penalty term) to get optimality. (This idea was originally presented in Christoph Lehrenfeld's Diploma Thesis [2010] under the direction of

Joachim Schöberl) Preliminary numerical results on polygonal meshes are presented.

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MS10

An Exponentially Convergent Iterative Solver for HDG Discretization of Partial Differential Equations

We present a scalable and efficient iterative solver for high-order hybridized discontinuous Galerkin (HDG) discretizations of hyperbolic partial differential equations. It is an interplay between domain decomposition methods and HDG discretizations. In particular, the method is a fixed-point approach that requires only independent element-by-element local solves in each iteration. As such, it is well-suited for current and future computing systems with massive concurrencies. We rigorously show that the proposed method is exponentially convergent in the number of iterations for transport and linearized shallow water equations. Furthermore, the convergence is independent of the solution order. Various 2D and 3D numerical results for steady and time-dependent problems are presented to verify our theoretical findings.

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MS10

H-to-P Efficiently: Solving HDG Systems via AMG Within The Nektar++ Framework

Complex finite element software is necessary to meet the demands of some of todays most challenging computational problems. The design of software is therefore more important than ever to ensure correctness of the results and manageability and sustainability of the implementation. We illustrate the approach taken within the Nektar++ spectral/hp element framework to compartmentalize code to align with the mathematical description and to produce a software solution which retains performance and platform portability. In this talk, we focus on our efforts to implement and solve hybridized discontinuous Galerkin (HDG) systems using a smoothed aggregation-based Algebraic Multigrid (AMG) solver for the HDG trace system. Since the globally coupled unknowns are traces on the mesh skeleton, the HDG approach essentially reduces the dimensionality of the problem by one, and hence minimizes the number of coupled unknowns. This makes it challenging to obtain good parallel scalability on large systems. We also present early scalability results from a parallel implementation of the AMG solver, by ensuring sparsity at coarser grids.

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MS11

G-Crossed Braided Fusion Categories and (3+1)-TQFTs

Higher categories are a rich source for constructing TQFTs. We show that with a G-crossed braided fusion category one can construct a non-trivial Turaev-Viro type (3+1)-TQFT. The partition function of a 4-manifold is written as a state sum on a triangulation of the 4-manifold. The 4-manifold invariants obtained this way generalize several known invariants in literature such as the Crane-Yetter invariant and Dijkgraaf-Witten invariant. Connections with other invariants will also be addressed.

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MS11

Exact Sequences of Tensor Categories with Respect to a Module Category

We generalize the definition of an exact sequence of tensor categories due to Bruguieres and Natale, and introduce a new notion of an exact sequence of (finite) tensor categories with respect to a module category. We give three definitions of this notion and show their equivalence. In particular, the Deligne tensor product of tensor categories gives rise to an exact sequence in our sense. We also show that the dual to an exact sequence in our sense is again an exact sequence. This generalizes the corresponding statement for exact sequences of Hopf algebras. Finally, we show that the middle term of an exact sequence is semisimple if so are the other two terms.

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MS11

Modular Extensions of Braided Fusion Categories and their Group Structure — from the Categorical Classification of 2+1D SETs

We propose that 2+1D topological orders with symmetry $\mathcal{E} = \mathrm{Rep}(G)$ or $\mathcal{E} = \mathrm{sRep}(G^f)$ (SETs) are classified by non-degenerate unitary braided fusion categories over the symmetric fusion category $\mathcal{E}$ ($\mathrm{UMTC}_{/\mathcal{E}}$), together with their modular extensions. Based on this proposal, the physical intuitions motivate a nice mathematical construction for a monoidal structure of the modular extensions, which corresponds to physically stacking layers of topological phases. We will introduce this construction and show that the modular extensions $\mathcal{M}_{ext}(\mathcal{E})$ of the symmetric fusion category $\mathcal{E}$ form an abelian group. Moreover, they act on the modular extensions $\mathcal{M}_{ext}(\mathcal{C})$ of a UMTC$_{/\mathcal{E}}$ $\mathcal{C}$ freely and transitively; in other words, $\mathcal{M}_{ext}(\mathcal{C})$ form a $\mathcal{M}_{ext}(\mathcal{E})$-torsor.

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MS11

On Gauging Symmetry of Modular Categories

Topological order of a topological phase of matter in two spacial dimensions is encoded by a unitary modular (tensor) category (UMC). A group symmetry of the topological phase induces a group symmetry of its corresponding UMC. Gauging is a well-known theoretical tool to promote a global symmetry to a local gauge symmetry. In this talk we will discuss several foundational problems, their mathematical formulations aand some applications, such as the relation with quantum computation. We will also present some recent results we have obtained. In particular, we will give a mathematical formulation of gauging in terms of higher category formalism. Roughly, given a UMC with a symmetry group G, gauging is a 2-step process: first extend the UMC to a G-crossed braided fusion category and then take the equivariantization of the resulting category. Gauging can tell whether or not two enriched topological phases of matter are different, and also provides a way to construct new UMCs out of old ones.

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MS12

Analytic Properties of the Dirichlet to Neumann Map for Electromagnetism

The electrodynamic response of any inhomogeneous body is governed by the frequency dependent Dirichlet to Neumann map. If instead to looking at the map which takes the tangential electrical field to the tangential magnetic field, one looks at the map which takes the tangential electrical field to the cross product of the normal to the body and the magnetic field, then we prove this is a operator valued Herglotz function of the component moduli (permittivities and permeabilities) multiplied by the frequency that is analytic when these products all lie in the upper half of the complex plane. As a result the Dirichlet to Neumann map has an integral representation and one can derive universal bounds limiting the transient or time-harmonic electrodynamic response of bodies. We anticipate that using these bounds in an inverse way will lead to entirely new methods for imaging what is inside a body. This joint work is Chapter 4 of the new book "Extending the Theory of Composites to Other Areas of Science" edited by Graeme W. Milton, and published by Milton-Patton Publishing.

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MS12

Radiative Transport and Scattering of Entangled Two-Photon States

We consider the scattering of entangled two-photon states from deterministic and random media. We show that the Wigner transform of the two-photon amplitude obeys an equation that is analogous to the radiative transport equation for classical light. Using this result, we calculate the entropy of entanglement and investigate the influence of the entanglement of the incident field on the entanglement of the scattered field.

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MS12

Nonlinear Optics with Balanced Gain and Loss

Nonlinear optics in media with balanced gain and loss is a research frontier of optics nowadays. Loss was used to be considered as a detrimental physical effect which should always be suppressed. But recent research shows that, by judiciously introducing loss to balance gain, such as in parity-time (PT) symmetric configurations, new optical devices such as single-mode PT lasers can be invented.

The novelty of optical systems with balanced gain and loss is that these systems are dissipative by nature, yet they behave much like conservative systems, which is very surprising. In this talk, we review nonlinear properties of light propagation in optical media with balanced gain and loss, including PT-symmetric and non-PT-symmetric configurations. Some challenging mathematical questions will also be pointed out.

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MS13

Non-Polynomial Discretization Schemes for Wave Problems Are Often Ill-Conditioned: Why?

The simulation of wave problems at high frequencies typically requires a large number of degrees of freedom. A range of modern numerical methods aim to reduce that number, often via novel discretization schemes. Many of these schemes lead to severely ill-conditioned discretization matrices, yet they also achieve highly accurate solutions. In this talk we aim to explain that apparent contradiction. In our analysis we focus on the *redundancy* in these discretizations, and we fully analyze the simpler problem of approximating functions using redundant sets.

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MS13

Generalized Plane Waves for Inhomogeneous Media Wave Propagation

Abstract Not Available at Time of Publication

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MS13

BEM/FEM Coupling for Transient Acoustic Scattering by Piezoelectric Obstacles

A coupled BEM/FEM formulation for transient acoustic scattering by piezoelectric obstacles is proposed. The acoustic wave is represented by retarded layer potentials while the elastic displacement and electric potential are treated variationally, resulting in an integro-differential system. Well posedness of the Galerkin semi-discretization is shown in the Laplace domain and translated into time domain bounds. Trapezoidal-Rule and BDF2 Convolution Quadrature are combined with time stepping for time discretization obtaining a second order scheme.

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MS13

Fast Algorithms for Oscillatory Integral Operators

In this talk, we will discuss some recent progress on butterfly algorithms for oscillatory integral operators and their applications to wave propagation problems.

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MS14

On the Complexity of Low-Rank Matrix Approximations

Given a matrix M, computing a rank-r approximation of M is a key problem and has many applications. Using the least-squares error, finding an optimal solution is equivalent to PCA and truncated SVD. We discuss in this talk the complexity of three variants: (i) nonnegative matrix factorization, (ii) robust PCA, and (iii) weighted PCA which can model missing data. Although these variants are NP-hard, we discuss several practical cases when they can be solved efficiently.

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MS14

Successive Rank-One Approximations of Nearly Orthogonally Decomposable Symmetric Tensors

Many idealized problems in signal processing, machine learning, and statistics can be reduced to the problem of finding the symmetric canonical decomposition of an underlying symmetric and orthogonally decomposable (SOD) tensor. Drawing inspiration from the matrix case, the successive rank-one approximation (SROA) scheme has been proposed and shown to yield this tensor decomposition exactly, and a plethora of numerical methods have thus been developed for the tensor rank-one approximation problem. In practice, however, the inevitable errors (say) from estimation, computation, and modeling necessitate that the input tensor can only be assumed to be a nearly SOD tensor—i.e., a symmetric tensor slightly perturbed from the underlying SOD tensor. This paper shows that even in the presence of perturbation, SROA can still robustly recover the symmetric canonical decomposition of the underlying tensor. It is shown that when the perturbation error is small enough, the approximation errors do not accumulate with the iteration number. Numerical results are presented to support the theoretical findings.

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MS14

Sparse Hierarchical Tucker Factorization and its Application to Healthcare

We propose a new tensor factorization method, called the Sparse Hierarchical-Tucker (Sparse H-Tucker), for sparse and high-order data tensors. Sparse H-Tucker is inspired by its namesake, the classical Hierarchical Tucker method, which aims to compute a tree-structured factorization of an input data set that may be readily interpreted by a domain expert. However, Sparse H-Tucker uses a nested sampling technique to overcome a key scalability problem in Hierarchical Tucker, which is the creation of an unwieldy intermediate dense core tensor; the result of our approach is a faster, more space-efficient, and more accurate method. We test our method on a real healthcare dataset, which is collected from 30K patients and results in an 18th order sparse data tensor. Unlike competing methods, Sparse H-Tucker can analyze the full data set on a single multi-threaded machine. It can also do so more accurately and in less time than the stateof-the-art: on a 12th order subset of the input data, Sparse HTucker is 18 more accurate and 7.5 faster than a previously state-of-the-art method. Moreover, we observe that Sparse HTucker scales nearly linearly in the number of non-zero tensor elements. The resulting model also provides an interpretable disease hierarchy, which is confirmed by a clinical expert.

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MS14

Generalized Low Rank Models

Abstract Not Available at Time of Publication

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MS15

Pilot-Wave Hydrodynamics

A decade ago, it was discovered that a millimetric droplet may self-propel across the surface of a vibrating bath by virtue of a resonant interaction with its own wave field. This hydrodynamic system is unique in that it exhibits several features previously thought to be exclusive to the microscopic, quantum realm. I review work in the experimental and theoretical modeling of this hydrodynamic pilot-wave system, and its relation to realist models of quantum dynamics.

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MS15

A PDE of Variational Electrodynamics

The electromagnetic two-body problem is an infinite-dimensional problem with four state-dependent delays of neutral type, with solutions that can be periodic orbits with discontinuous velocities. Continuous maps of light-cone type from R^4 to points along such periodic orbits naturally inherit the derivative discontinuities and our distributional construction to accomodate such discontinuities involves a second order PDE. We will discuss the distributional construction and the importance of such PDE to variational electrodynamics.

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MS15

Delay ODE's and PDE's in Classical and Quantum Electrodynamics

Due to the finite speed of light, differential equations involving delay appear naturally in electrodynamics. Classical electrodynamics in terms of charges and fields is usually described by a coupled system of ODEs and PDEs without delay, effective ODEs involving delay emerge as soon as one attempts a mathematical rigorous treatment of radiation reaction. I will discuss the famous equations of Dirac, Synge, and Wheeler and Feynman and how PDEs with delay occur in the mean-field description of quantum electrodynamics. Although the discussed ODE and PDE settings are quite different, they share the same basic obstacle: With unbounded, state-dependent delay, the notion of local solution ceases to make sense. Standard techniques usually fail and one needs to fall back to topological fixed-point arguments to ensure global existence.

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MS15

State Dependent Delays in the Biological Sciences: Where Do They Come From?

Biological systems often have dynamics in which delays play a significant role. These delays may be state-dependent (either increasing or decreasing functions of the state variable) or distributed, or both. This talk will survey some of the many examples in the biological sciences in which this occurs, how those delays arise as well as their nature. Examples will be drawn from neurobiology, cell biology, and molecular biology.

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MS16

Transcriptomics of Bleaching and Recovery in the Alcyonacean Octocoral Sympodium Sp.

Worldwide, coral reefs are being threatened by coral bleaching, a potentially lethal stress response. Despite much research on bleaching in scleractinian (reef-building) corals and the model organism *Aiptasia*, our understanding of bleaching in octocorals (soft corals and sea fans) is limited. To resolve this, we have sequenced and assembled transcriptomes of the octocoral *Sympodium* sp. and its endosymbionts at key time points in the bleaching process, and are analyzing changes in gene expression patterns. Advisor: Daniel Martinez, Pomona College

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MS16

Bounds for Bond Percolation Thresholds of Archimedean Lattices

Abstract Not Available at Time of Publication Advisor:

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MS16

Analysis of Individual Greensboro Police Officers Stopping Patterns Using Propensity Score Weighting

Due to allegations of racial profiling during traffic stops, the Greensboro Police Department requested an analysis of traffic stops in similar neighborhoods during concurrent time periods in order to identify officers who disproportionately stop African Americans. The RAND Corporation's methodology with propensity score weighting and false discovery rates was utilized for this analysis. Results showed there was a high probability that 10 out of the 563 officers racially profiled African Americans during traffic stops. Advisor: Jan Rychtr, University of North Carolina at Greensboro.

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MS16

On an Empirical Analysis of the Kidney Allocation System

We conduct an empirical study of dynamic choice in the kidney allocation system. We find that the newly implemented system, which prioritizes candidates with high antibody sensitivity, has a significant effect on acceptance probability and offer rates because of adjusted expectation in arrival rate. Advisor: Robert Langer, MIT

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MS16

Strategies to Eliminating Space Debris: Approaches from a Time-depentent Evaluation Model

In this MCM problem, we reduced the spatial problem into a 2D probability model and employed gamma distribution to simulate the space debris distribution, to evaluate the potential commercial opportunity for a satellites insurance provider. A third party, policy makers, is also discussed with a game theory approach. According to our results, the insurance commission fee shall exceed 4% of each launch cost, and both land and spatial removal approaches shall be employed to attain the optimal outcome. Relevant sensitivity tests are also conducted. Advisor: Professor Dai Dai, Southwestern University of Finance and Economics, China

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MS16

Dynamics of Atomtronic Battery

Atomtronics studies cold atom analogues of electronic circuits. An ultra-cold Bose gas cloud trapped in a specially shaped trap can serve as a "battery' for such a circuit. We investigate the behavior of this system at different loads. We first perform a bifurcation analysis with respect to the adjustable out-coupling parameter and find a domain where stable solutions exist, as well as a range of initial conditions that converge to stable equilibria. We also look at the relation between the load current and chemical potential, which gives the I-V relation of the battery, and find that the model resembles an electronic battery well at low loads, but shows negative resistance at high loads. Advisors: Burt Tilley, Dept. of Mathematical Sciences, WPI Alex Zozulya, Dept. of Physics, WPI

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MS17

Student Presentations TBA

During the spring 2016 semester, mathematical sciences undergraduate students at 50 U.S. universities and colleges were enrolled in a PIC Math (Preparation for Industrial Careers in Mathematical Sciences) industrial mathematics and statistics research course. Each student team worked on a research problem, which came directly from industry, and submitted a written report and video solution to the problem to the PIC Math student research competition. Several students will give a presentation of their problem and solution during this session. PIC Math is a program of the MAA and SIAM supported by NSF funding (DMS-1345499). See http://www.maa.org/picmath

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MS18

PIC Math Industry talk 2 - To Be Announced

Abstract Not Available at Time of Publication

To Be Announced
Industry 2
tba

MS18

PIC Math Industry talk 1 - To Be Announced

Abstract Not Available at Time of Publication

To Be Announced
Industry 1
tba

MS19

Algebraic Statistics of Gaussian Mixtures

Gaussian mixture models have a rich history in statistics, with a wide range of applications. A key question for such models is how to learn the defining parameters from a data sample. In this talk, we will explore some theoretical and computational consequences for this inference problem by studying and comparing solutions based on method of moments and maximum likelihood from an algebraic geometry perspective. Based on ongoing joint work with Mathias Drton, Jean-Charles Faugere and Bernd Sturmfels.

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MS19

What Is the Shell Distribution of a Graph Telling Us?

The k-core of a graph is its largest subgraph such that all nodes have degree at least k in the subgraph. The shell index of a node, the largest core it belongs to, can be used a measure of importance of a node. We propose to model networks by their shell structures and discuss network models based on the core decomposition of a graph.

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MS19

Tensor Completion in the Probability Simplex

We study the rank one tensor completion in the probability simplex from the algebro-geometric perspective. Given a pattern of observed entries, the set of partially observed tensors that can be completed to rank one tensors in the probability simplex form a semialgebraic set. We study the semialgebraic description and algebraic boundary of this semialgebraic set for different patterns of observed entries. This is joint work with Thomas Kahle, Mario Kummer and Zvi Rosen.

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MS19

Positive Semidefinite Rank and Nested Spectrahedra

The set of matrices of given positive semidefinite rank is semialgebraic. In this work we study its geometry and in small cases we describe its boundary. For general psd rank we give a conjecture for its boundary and for its semialgebraic description. Our proof techniques are based on studying nested spectrahedra and spectrahedral shadows.

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MS20

A Mathemaical Model of the Effects of Temperature on Human Sleep Patterns

Several studies have been done on human patients that suggest that different temperatures, such as room temperature, core body temperature, and distal skin temperature, have an important effect on sleep patterns, such as length and frequency of REM bouts. A mathematical model is created to investigate the effects of temperature on the REM/NonREM dynamics. Our model was based on previous well established and accepted models of sleep dynamics and thermoregulation models.

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MS20

Modeling Respiratory Dynamics in the Premature Infant

The survival rate for very premature infants is increasing, but these babies are at significant risk for developing chronic lung disease as a consequence of exposure to mechanical ventilation. Increased compliance (flexibility) of the chest wall due to early gestation bone undermineralization results in progressive lung collapse as the forces needed to open airspaces after each exhalation become insufficient. We present a mathematical model of respiratory dynamics in premature infants that accounts for changes in chest wall compliance, with the ultimate aim of developing a treatment that increases chest wall rigidity to allow for mechanical ventilation.

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MS20

Modeling Autoregulation in the Kidney

Autoregulation refers to the ability of vascular beds to maintain nearly constant blood flow despite large fluctuations in blood pressure. Impaired autoregulation in the kidney is both a symptom and contributing factor in diseases such as hypertension and diabetes. The model presented here couples two autoregulation mechanisms, generating new insight into how blood flow in the kidneys of healthy and diabetic patients changes in response to increased blood pressure or impaired regulatory mechanisms. (Joint work with J. C. Arciero, L. Ellwein, A. N. Ford Versypt, and A. T. Layton)

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MS20

Using Delayed Feedback to Avoid Neural Synchrony

The spontaneous synchronization of certain groups of neurons is responsible for epileptic seizures as well as some of the motor symptoms of Parkinsons Disease. Breaking neural synchrony through deep brain electrical stimulation is a key method of treatment of these conditions. We will discuss the mathematics of how synchrony can be avoided in dynamic networks. In particular, we will highlight how time-delayed linear feedback can be used to avoid synchrony in an artificial neural network.

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MS22

Data-Driven Identification of Nonlinear Dynamical Systems with Control using Sparse Regression

This work develops a general framework to discover dynamical system from data using sparse regression. The resulting models are parsimonious, balancing model complexity with descriptive ability while avoiding overfitting. The only assumption about model structure is that there are relatively few terms governing the dynamics, so the equations are sparse in the space of possible functions. We also connect this method with dynamic mode decomposition (DMD) and Koopman analysis in the broader context of dynamic regression.

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MS22

In-Situ Analytics in Extreme Scale Combustion Simulations

In situ analytics and visualization in turbulent combustion simulations are enabled by Legion, a dynamically scheduled task-based parallel programming model and runtime system for hybrid architectures. By inferring task dependences, the Legion runtime automatically manages all of the data movement making it simpler to modify, port and remap computation and analytics kernels from GPU's to CPU's. In situ chemical explosive mode analysis, used to assess properties of reaction rates in real time, is used to guide in situ visualization.

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MS22

Data-Driven Coarse-Graining for Multiscale Problems

Abstract Not Available at Time of Publication

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MS22

Inferring Interaction Rules from Observations of Evolutive Systems

In this talk we are concerned with the learnability of nonlocal interaction kernels for first order systems modeling certain social interactions, from observations of realizations of their dynamics. In particular, we assume here that the kernel to be learned is bounded and locally Lipschitz continuous and that the initial conditions of the systems are drawn identically and independently at random according to a given initial probability distribution. Then the minimization over a rather arbitrary sequence of (finite dimensional) subspaces of a least square functional measuring the discrepancy from observed trajectories produces uniform approximations to the kernel on compact sets. The convergence and its rate are obtained by combining mean-field limits, transport methods, and a Γ-convergence argument. A crucial condition for the learnability is a certain coercivity property of the least square functional, majoring an L_2-norm discrepancy to the kernel with respect to a probability measure, depending on the given initial probability distribution by suitable push forwards and transport maps. We illustrate the convergence result by means of several numerical experiments.

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MS23

Mathematical Foundations of the GraphBLAS

Sparse matrix representations of graphs rely on a few key matrix operations. These include element-wise addition, element-wise multiplication, scalar multiplication, and matrix multiplication. GraphBLAS matrices map rows and columns to a value set that is equipped with two binary operations $\oplus$ and $\otimes$. The global properties of the matrix operations are determined by the local properties of the value set. These properties are connected via abstract algebra concepts such as zero-sum-free semi-rings that form the foundation of the GraphBLAS.

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MS23

Design and Implementation of the GraphBLAS Template Library (GBTL)

An important design goal of GBTL is to achieve a separation of concerns between graph algorithm development and performance tuning required for various heterogeneous high-performance computing (HHPC) architectures. In GBTL, the GraphBLAS API specifies the primitive operations and data structures that allow this separation of concerns. We implement this API for both generic CPU systems and GPU systems, and present a number of important graph algorithms written in terms of this API.

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MS23

GraphMat: Increasing Productivity and Performance for Large Graph Problems using Distributed Primitives

We describe the design and implementation of GraphMat, our distributed graph processing framework based on GraphBLAS primitives that provides a productive vertex programming frontend. Our framework can flexibly accommodate different data structures such as CSR and DCSC for storing graphs as well as different partitioning strategies such as 1D, 2D-block and 2D-block-cyclic schemes. We show that GraphMat has better performance than other graph frameworks and works efficiently on both HPC and cloud platforms without compromising productivity.

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MS23

Task Parallel Approach to the Linear Algebra-Based Implementation of miniTri

Recently, we developed a triangle enumeration-based data analytics miniapp, which mimics the computation requirements of an important set of data science applications, not well represented by traditional benchmarks. Here, we describe an asynchronous, task parallel approach that enables our linear algebra-based implementation of miniTri to process significantly larger graphs and is potentially beneficial to the larger GraphBLAS effort. We describe our experiences with improving the efficiency of this task parallel implementation and present performance results.

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MS24

Preconditioning from a Single Matvec

This talk introduces a preconditioner constructed via a single matrix-vector multiplication according to the feature of the given structured matrix.

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MS24

Approximate Cholesky Factorization for Laplacians Fast, Sparse, and Simple

We present a simple, nearly linear time algorithm that computes a sparse approximate Cholesky factorization of a Laplacian matrix. This gives the first efficient solver for Laplacian systems that is based purely on random sampling, and does not use any graph theoretic constructions such as low-stretch trees, graph sparsifiers, or expanders. The crux of our analysis is a novel concentration bound for matrix martingales whose differences are sums of conditionally independent variables.

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MS24

Distributed-Memory Hierarchical Interpolative

Factorization

In this talk, we propose a distributed-memory algorithm for the hierarchical interpolative factorization, which is a novel framework for efficient solution of partial differential equations and integral equations. The implementation can be applied to three-dimensional most elliptic problems as well as low-to-medium frequency hyperbolic problems. Numerical experiments demonstrate that these problems with almost billions of unknowns can be efficiently solved with thousands of processes in minutes.

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MS24

Fast Likelihood Evaluation Using Hierarchical Matrices in Bayesian Inverse Problems

MCMC approaches to Bayesian inverse problems require repeated evaluation of (ratios of) the log likelihood of the posterior distribution. For inverse problems with many measurements, this can easily involve upwards of 10^6 PDE solves. We use the Hierarchical matrix approach combined with randomized algorithms to reduce the computational cost associated with likelihood evaluation. The resulting computational benefits will be demonstrated on a challenging model problem in Diffuse Optical Tomography.

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MS25

Hybridizable Discontinuous Galerkin Methods for Elastodynamics

In this talk we will present some preliminary results on the use of an HDG method for the simulation of elastic waves. We will show how the Qiu and Shi choice of spaces and stabilization parameters for an HDG scheme applied to quasistatic elasticity also apply for time harmonic elastic waves, providing a superconvergent method. We will next discuss a conservation of energy property that holds in the transient case when the elasticity equations are semidiscretized in space with the same HDG strategy. We will finally show some numerical experiments in three dimensions.

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MS25

High order exactly Divergence-Free HDG Methods for Incompressible Flows

For the discretization of unsteady incompressible Navier-Stokes equations we consider operator splitting combining the efficient numerical treatment of hyperbolic transport and a Stokes-type problems. In the considered splitting the implicit treatment of the Stokes part involves the solution of linear systems. We consider an HDG discretization for this with two important features: $H(\mathrm{div})$-conforming finite elements and a projection operator which reduces the number of globally coupled unknowns.

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MS25

Hybridizable Discontinuous Galerkin Methods for Coastal Ocean Dynamics

We discuss high-order Finite-Element schemes and codes that combine the Hybridizable Discontinuous Galerkin (HDG) method, projection methods, and Implicit-Explicit Runge-Kutta (IMEX-RK) time-integration schemes. The application focus is non-hydrostatic ocean physics including a nonlinear free-surface and coastal biogeochemical dynamics. Implementations are tested and verified using the method of manufactured solutions and benchmark test cases. Results of numerical convergence studies are shown. Specific attention is given to the IMEX-RK time-integration, pressure iterations and selective limiters.

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MS25

Construction and Analysis of Hybridized Discontinuous Galerkin Methods for the Magnetohydrodynamics Equations

Inspired by the upwind HDG framework, we systematically construct and analyze HDG methods for linearized resistive magnetohydrodynamics equations. The framework consists of first deriving upwind-type numerical fluxes and then hybridizing them. From this perspective, we can view an HDG method as a DG approach with a hybridized flux. We prove well-posedness and analyze *a priori* error convergence associated with our HDG formulations. Various 2D and 3D numerical results are presented for both steady state and unsteady problems.

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MS26

Variable Projection in Nonsmooth Applications

Variable projection is a popular technique for solving structured nonlinear optimization problems, where decision variables can be naturally partitioned into two blocks (and one block can be 'projected' out). We describe classic formulations and the approach, and then show that the idea extends nicely to new contexts in large scale learning, with numerous applications including PDE constrained optimization, nuisance parameter estimation, statistically robust techniques, multiple kernel learning, and nonsmooth regularizations of classic formulations.

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MS26

SMART: The Stochastic Monotone Aggregated Root-Finding Algorithm

We introduce the Stochastic Monotone Aggregated Root-Finding (SMART) algorithm, a new randomized operator-splitting scheme for finding roots of finite sums of operators. These algorithms are similar to the growing class of incremental aggregated gradient algorithms, which minimize finite sums of functions; the difference is that we replace gradients of functions with black-boxes called operators, which represent subproblems to be solved during the algorithm. By replacing gradients with operators, we increase our modeling power, and we simplify the application and analysis of the resulting algorithms. The operator point of view also makes it easy to extend our algorithms to allow arbitrary sampling and updating of blocks of coordinates throughout the algorithm. Implementing and running an algorithm like this on a computing cluster can be slow if we force all computing nodes to be synched up at all times. To take better advantage of parallelism, we allow computing nodes to delay updates and break synchronization.

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MS26

Expanding the Reach of Optimal Methods

First order methods with optimal convergence rates for smooth convex minimization have had a profound impact on computation. Such optimal methods, however, lack intuition. I will begin by describing an intuitive optimal method for minimizing strongly convex functions, rooted in elementary cutting plane ideas. Without convexity, best-known complexity bounds worsen to those achieved by simple gradient descent. In the second part of the talk, I will present a new optimal method for minimizing compositions of convex and smooth functions that is agnostic to convexity. The resulting scheme is closely related to the proximal gradient method, FISTA, and the Gauss-Newton algorithm. A natural convexity parameter of the composition governs the transition between the best known rates for convex and for nonconvex problems that the algorithm achieves.

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MS27

Classical Spin Models with Global Symmetries and Quantum Models with Local Symmetries

We generalize the duality between classical lattice spin systems with global abelian symmetries and quantum systems with local symmetries. The classical systems have symmetries associated with subsets of the lattice. The dual quantum systems exhibit ground state degeneracy and gapped energy spectrum that are robust under arbitrary perturbations, but might not have a topological quantum field theory analog.

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MS27

Constraints on Multiparticle Entanglement

States of a multiparticle quantum system are useful for quantum information processing when they are entangled. Arbitrary entanglements between parts of a quantum system are not possible, however; they must satisfy certain "monogamy' constraints which limit how much multiple different subsystems can be entangled with one another. In this talk we'll generalize the standard monogamy constraints in several ways. The tools we use to obtain these results include Gröbner basis calculations and linear matrix inequalities.

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MS28

The Fascinating Optics of Metamaterials and Plasmonics

Metamaterials and plasmonics offer unprecedented opportunities to tailor and enhance the interaction of waves with materials. In this talk, I discuss our recent research activity in electromagnetics and nano-optics, showing how suitably tailored meta-atoms and suitable arrangements of them open exciting venues to manipulate and control waves in unprecedented ways. I will discuss our recent theoretical and experimental results, including nanoclusters and metasurfaces to control wave propagation and radiation, large nonreciprocity without magnetism induced by nonlinearities and temporal modulation, large nonlinearities in tailored metamaterials, and parity-time symmetry in meta-atoms and metasurfaces with gain. Physical insights into these exotic phenomena, new devices based on these concepts, and their impact on technology will be discussed during the talk.

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MS28

On the Homogenization of a Transmission Problem in Scattering Theory for Highly Oscillating Periodic Media

We discuss the homogenization of a transmission problem arising in the scattering theory for bounded inhomogeneities with periodic coefficients modeled by the anisotropic Helmholtz equation. The coefficients are assumed to be periodic functions of the fast variable, specified over the unit cell with small characteristic size. By way of multiple scales expansion, we establish higher-order bulk and boundary corrections of the leading-order homogenized transmission problem. The analysis in particular provides rigorous estimates of the error committed by the first-order-corrected solution considering both boundary and bulk correction. We also present explicit boundary corrections for the transmission problem when the scatterer is a unit square and its limit as the cell size goes to zero. At the end we briefly consider the homogenization of the corresponding transmission eigenvalue problem and show that the transmission eigenvalues, which can be determined from the scattering data, can be used to reconstruct the effective material properties of the highly oscillating periodic media. This is joint work with B. Guzina and S. Moskow.

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MS28

Free Form Optical Design and Monge-Ampere Type Equations

I will describe models and recent results concerning the mathematical design of a surface separating two materials with different refractive indices that refracts radiation emanating from a point source with a given energy distribution into a given target with a prescribed distribution of energy to be received. Questions concern existence, uniqueness and smoothness properties of the surface solutions. The techniques used are from optimal mass transport, optimization, and nonlinear partial differential equations of Monge-Ampere type. The equations appear naturally because the ratio between the energy sent and received over a small aperture can be expressed in terms of the input and output given energies. I will also outline an algorithm that can be implemented to solve the problem numerically.

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MS28

Embedded Eigenvalues in Electromagnetic Structures

This presentation will discuss the mathematics and applications of eigenvalues of photonic systems that are embedded in the continuum of extended states. Such an eigenvalue could correspond, for example, to an exponentially bound state in a defective waveguide or to a guided mode along a periodic waveguide that is open to an ambient space. The significance of an eigenvalues being embedded lies in its instability. This means that a generic perturbation of the system causes the eigenvalue to dissolve and allows extended states effectively to couple resonantly with the bound state. This resonance can be viewed either as an impediment to the functionality of a photonic device or as an integral part of its design. Typically, an embedded eigenvalue is a result of a symmetry of the system, which produces invariant subspaces with different continuous spectrum. A non-embedded eigenvalue for one invariant space can be embedded in the continuum of the other. Analysis shows that an embedded eigenvalue that is not associated to a symmetry of the system would possess useful detuning properties. There is evidence that such asymmetric eigenvalues exist in photonic wave-guide structures, and it can be shown that they do exist for bilayer graphene with a localized defect. The presentation will discuss current investigations involving embedded eigenvalues and highlight the issues of topological protection, asymmetry, and reciprocity.

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MS29

Advances in Optimized Fourier Continuation Methods

Recent advances in techniques for improved performance of Fourier Continuation/Extension methods for the solutions of PDEs will be discussed. The stability of these algorithms have been outstanding, yet the methodology allows even greater performance if the stability can be better controlled in more extreme cases. Various strategies used to stabilize Fourier Continuation methods will be compared with new approaches.

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MS29

High-Frequency Asymptotic Compression of Dense BEM-Matrices

A BEM discretization matrix A for a Helmholtz problem is typically large, dense and ill-conditioned for high wavenumbers. We modify the Green's function using C^∞ windowing functions in an otherwise standard BEM implementation, since interactions become local at high frequencies. The locations of these windows can be computed automatically for general 2D and 3D geometries. This introduces sparsity in A and reduces the condition number.

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MS29

A Fast Hierarchical Direct Solver for Singular Integral Equations Defined on Disjoint Boundaries and

Application to Fractal Screens

A fractal antenna uses a self-similar design to achieve excellent broadband performance. Similarly, a fractal screen has surprising numerical properties that we explore with a hierarchical solver. We consider a recursive block LU factorization designed to exploit the strong admissibility implied by the boundary integral formulation of elliptic partial differential operators. The hierarchical solver involves a pre-computation phase independent of the right-hand side. Once factored, the solution for multiple inputs exhibits even lower complexity.

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MS29

Breaking the $\mathcal{O}(N)$ Barrier for High-Frequency Helmholtz Equation

We present a new fast and scalable algorithm to solve the 3D high-frequency Helmholtz equation in heterogeneous medium for multiple right-hand sides. The algorithm relies on domain decomposition, integral operators, and an efficient pipelining to achieve an asymptotic runtime $\mathcal{O}(N \max(1, R/n))$, where R is the number of right-hand sides and $N = n^3$ the number of degrees of freedom.

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MS30

Heterogeneous and Vectorized Computation for Quantum Chemistry

To efficiently utilize upcoming computer platforms, quantum chemistry algorithms and software must be able to use more and more parallelism. We discuss heterogeneous Hartree–Fock calculation on CPUs and Intel Xeon Phi. We also present the horizontal vectorization of electron repulsion integrals. This is joint work with Benjamin Pritchard, Xing Liu, and the Intel Parallel Computing Lab.

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MS30

Overview and Contrast of Modern Computer Architectures Including the Intel Phi

State-of-the-art distributed-memory clusters today contain multi-core CPUs with 8 to 12 cores, massively parallel GPUs with thousands of computational cores, and many-core accelerators such as the 60-core Intel Phi, connected by high-performance networks such as InfiniBand interconnect. This talk will give an overview of their features, discuss the possible modes and programming models, and contrast performance results for basic test problems.

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MS30

Improving Performance of Sparse Triangular Solution on GPUs and CPUs for Irregular Matrices

We seek to speedup Sparse-Triangular-Solution (STS) scheme for irregular matrices on GPUs and CPUs. We proposed a multilevel CSR (CSR-k) format to store a sparse matrix in a cache friendly manner on NUMA architectures. We formulate STS using CSR-k to expose more parallelism as compared to traditional schemes for irregular matrices and utilize the tremendous amount of thread-based parallelism present in GPUs. We evaluate the performance of our method on both GPU and CPU architectures.

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MS30

Porting and Tuning Numerical Kernels to Many-Core Intel Xeon Phi Accelerators

Modern architectures with multiple memory hierarchies in multi-core CPUs and coprocessors such as the massively parallel GPGPU and many-core Intel Xeon Phi offer opportunities to drastically speed up numerical kernels. We report the performance of test problems whose structure is representative of kernels of real-world application codes: the classical elliptic test problem of a Poisson equation with homogeneous Dirichlet boundary conditions in two and three dimensions.

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MS31

LP vs SDP Lifts of Polytopes

Nonnegative factorizations play an important role in the study of LP lifts of polytopes. Similarly positive semidefinite factorizations are directly related to SDP lifts. In this talk we are interested in comparing LP and SDP lifts. We construct an explicit family of polytopes in increasing dimensions where the SDP extension complexity is vanishingly smaller than the LP extension complexity.

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MS31

Coordinate Descent Methods for Matrix Factorization

Given a symmetric nonnegative matrix A, symmetric nonnegative matrix factorization (symNMF) is the problem of finding a nonnegative matrix H, usually with many fewer columns than A, such that $A \approx HH^T$. SymNMF can be used for data analysis and in particular for various clustering tasks. In traditional NMF or simply low-rank matrix factorization, typical methods like ALS or greedy coordinate descent separate the problem into a series of quadratic(convex) subproblems, which is not so computational efficient. We on the contrary propose to solve SymNMF by directly solving the non-convex problem, namely, minimize $\|A - HH^T\|^2$, which is a fourth-order non-convex problem. We propose simple and efficient coordinate descent schemes, which solve a series of fourth-order univariate subproblems exactly. We also derive convergence guarantees for our methods, and show that they perform favorably compared to recent state-of-the-art methods on synthetic and real-world datasets, especially on large and sparse input matrices.

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MS31

A Projected Gradient Scheme for Separable NMF

An important special case of the nonnegative matrix factorization (NMF) problem arises from imposing the *separability condition* on the given data. In contrast to the general NMF problem, the imposed separability condition leads to a polynomial time solvable one, and the challenge is to design *noise robust* and *fast* algorithms for its solution. In this work we present an efficient first order scheme, discuss its robustness, and show some relations to other self-dictionary based regression problems.

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MS31

Exact NMF and Compact Extensions of N-Gons

For a m-by-n nonnegative matrix X and an integer r, the exact NMF problem aims to find an m-by-r nonnegative matrix W and an r-by-n nonnegative matrix H such that $X = WH$. The nonnegative rank of X is the smallest r for which an exact NMF exists. The extension complexity of a polytope equals the nonnegative rank of its slack matrix. In this talk, we discuss exact NMF algorithms for finding compact extensions of polygons.

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MS32

A Unified, Goal-Oriented, Hybridized Reduced Basis Method and Generalized Polynomial Chaos Algorithm for Partial Differential Equations with Random Inputs

The generalized Polynomial Chaos (gPC) method using stochastic collocation is one of the most popular computational approaches for solving partial differential equations (PDEs) with random inputs. The main hurdle preventing its efficient direct application for high-dimensional randomness is that the solution ensemble size grows exponentially in the number of inputs (the curse of dimensionality). In this paper, we design a weighted version of the reduced basis method (RBM) and synergistically integrate it into the gPC framework. The resulting algorithm is capable of speeding up the traditional gPC by orders of magnitude without degrading its accuracy. Perhaps most importantly, the relative efficiency improves as the parametric dimension increases demonstrating the potential of our method in significantly delaying the curse of dimensionality. Theoretical results as well as numerical evidence justify these findings.

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MS32

Gaussian Functional Regression for Model-Data Assimilation

We introduce a Gaussian functional regression (GFR) technique that integrates multi-fidelity models with model reduction to efficiently predict the input–output relationship of a high-fidelity model. The GFR method combines the high-fidelity model with a low-fidelity model to provide an estimate of the output of the high-fidelity model in the form of a posterior distribution that can characterize uncertainty in the prediction. A reduced basis approximation is constructed upon the low-fidelity model and incorporated into the GFR method to yield an inexpensive posterior distribution of the output estimate. As this posterior distribution depends crucially on a set of training inputs at which the high-fidelity model are simulated, we develop a greedy sampling algorithm to select the training inputs. Our approach results in an output prediction model that inherits the fidelity of the high-fidelity model and has the computational complexity of the reduced basis approximation. Numerical results are presented to demonstrate the proposed approach.

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MS32

The Certified Reduced-Basis Method for Darcy Flows in Porous Media

In this work we extend the RB method to solve problems of two-phase flows in porous media discretized with a cell-centered finite volume scheme. Our first step in this study is to develop an efficient reduced basis scheme for the pressure equation. Here our first test consists in approximating all the pressure fields obtained at the final time step according to the values of the water viscosity using a RB approach. An a posteriori error estimate is built giving an upper bound on the residual obtained when replacing the discrete solution by the RB approximation. As an illustration, numerical experiments performed on the SPE10 benchmark are presented.

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MS32

Proper Orthogonal Decomposition in Uncertainty Quantification of Complex Fluid Flows

In many engineering applications such as the flow control and optimization problems, one is interested in determining statistical information about the quantities of interest, given statistical information about the inputs. The brute-force numerical simulations of the flows can become computationally infeasible when complex flows are considered due to the appearance of small scales in the flow, the high dimension of uncertain parameters, etc. Therefore, we propose a goal-oriented proper orthogonal decomposition approach to reduce the dimension of the numerical simulation model of complex flows, then use a Gaussian process to model the difference of outputs between the reduced-order model and the full-order model. Numerical tests show the effectiveness of the proposed approach.

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MS33

Galerkin Finite-Element Method with Discontinuous Velocity Applied to the Two-Body Electromagnetic Variational Problem

Breaking points play an important role in neutral differential delay equations with state-dependent delays. Determining how the derivative discontinuities propagate along the solutions is a challenge for numerical and functional analysis. We will discuss a Galerkin finite-element method with discontinuous velocities applied to the variational boundary-value formulation of the advanced-retarded two-body problem of electrodynamics and discuss how this method is able to find the chain of possible breaking points along the trajectories.

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MS33

Periodic Solutions and Their Bifurcations in a Singularly Perturbed Differential Equation with Two State-Dependent Delays

We present a construction technique for the potentially discontinuous limiting profiles of periodic solutions in singularly perturbed state-dependent delay differential equations (DDEs) through continuous nested parameterisations. We apply this technique to a singularly perturbed DDE which has two linearly state-dependent delays to determine periodic solutions and their bifurcations in the singular limit. We show that these bifurcation structures persist close to the singular limit by studying the bifurcation structures numerically in that case.

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MS33

Resonance Phenomena of a Delay Differential Equation with Two State-Dependent Delays

I will present a numerical study of the dynamics of a differential equation with two delays. The associated constant delay DDE obtained by freezing the delays is linear and without recurrent dynamics. In the presence of the two state-dependent delay terms, the DDE is inherently nonlinear and has much more complicated dynamics. In particular, we study dynamical behavior driven by the existence of two parameter families of invariant tori. A semi-numerical analysis based in a normal form predicts the existence of torus bifurcations from which stable invariant tori families emerge. We investigate the behavior of these invariant tori with respect to two parameters trough return maps. We also find boundaries of Arnold tongues and indications of lost of normal hyperbolicity of the stable family.

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MS35

A Learning Approach for Computing Regularization Parameters for Tikhonov Regularization

Computing regularization parameters for Tikhonov regularization can be an expensive and difficult task, especially if multiple parameters or many solutions need to be computed in real time. In this work, we assume training data is available and describe an efficient learning approach for computing regularization parameters that can be used for a large set of problems. Several tests are performed for 1D and 2D examples showing the effectiveness of this approach.

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MS35

Estimating Singular and Generalized Singular Value Bases Using Noise Revealing Techniques

Image denoising and restoration algorithms use iterative Lp regularizers (IR) with embedded Tikhonov regularizers. We consider image corruption operators with underlying Kronecker product form and analyze determination of the effective solution basis using noise revealing techniques for the basis vectors in each dimension. Initial discussion focuses on SVD decompositions, extended to GSVD bases for use in IR image restorations. Aims include improving efficiency in calculation of the tensor product GSVD and in image restoration algorithms.

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MS35

Iterative Methods for Multi-Parameter, Multi-Data X-Ray Tomography

Motivated by security screening applications, we consider the problem of mapping material properties, mass density and the photoelectric coefficient, from energy resolved X-ray data for severely limited view systems. Ill-posedness is partially addressed by augmenting absorption data with observations of Compton scattered photons resulting in a non-linear forward. Our work focuses on developing a novel regularization method for stably recovering the photoelectric coefficient and an ADMM method for solving the resulting optimization problem.

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MS35

Weighted Least Squares for an Image Deblurring Inverse Problem

We consider image deblurring problem with Poisson data and additive Gaussian noise. The maximum likelihood functional for this model can be approximated by a weighted least squares problem with the weights depending on the computed data. However, the least squares solution is not robust if outliers occur. We propose a modification of the data fidelity function using the idea of robust regression and test the resulting method on data with various types of outliers.

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MS36

Multifidelity Uncertainty Quantification With Application to CFD

This work introduces a model reduction approach that exploits the low-rank structure of the solution of interest for fast propagation of high-dimensional uncertainties. To construct the low-rank approximation, the method utilizes a low-fidelity model to learn a reduced basis and an interpolation rule that can be used to generate an approximation of the high-fidelity solution. Different aspects of this model reduction approach will be illustrated through its application to a CFD problem

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MS36

Probabilistic Evaluation of Downhole Fluid Sampling via Fast Proxy Modeling

Downhole acquisition of fluid samples using a wireline formation tester is an integral part of characterizing a hydrocarbon reservoir. With inherent uncertainties in formation and fluid properties, probabilistic evaluations of sampling time are needed. In this paper, we show how high-fidelity proxies are built for the fluid sampling process. We demonstrate how the proxy models enable rapid quantification of uncertainty in sampling time and identifying parameters contributing substantially to this uncertainty through global sensitivity analysis.

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MS36

Quantifying the Impacts of Parametric Uncertainty in Biogeochemistry in the ACME Land Model

Large uncertainties remain in climate predictions, many of which originate from uncertainties in land-surface processes. In particular, uncertainties in land-atmosphere fluxes of carbon dioxide and energy are driven by incomplete knowledge about model parameters and their variation over space and time. Using the ACME land model, we perform uncertainty decomposition based on global Polynomial Chaos (PC) surrogate construction, using the Bayesian Compressive Sensing (BCS) sparse learning technique.

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MS36

Global Sensitivity Analysis for Large Eddy Simulation Models

The Large Eddy Simulation (LES) technique can potentially provide relatively accurate flow predictions for a variety of of flow configurations. For configurations of practical interest, however, this approach can be prohibitive due to the large number of model parameters and the large computational mesh required by the model. In this work we present a dimensionality reduction approach based on Global Sensitivity Analysis augmented with multifidelity and compressed sensing algorithms to eliminate unimportant parameters and design low-dimensional surrogate models for Quantities of Interest relevant to turbulent flows.

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MS37

Parallel Mixed Volume Computation Revisited

The concept of mixed volume plays an important role in the study of systems of polynomial equations via Bernshtein's Theorem and the polyhedral homotopy method of Huber and Sturmfels. In this talk we review some recent development in parallel algorithms for mixed volume computation as well as the revival of a few classical ideas.

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MS37

Numerical Algebraic Geometry and Synchronization of Coupled Phase Oscillators

The Kuramoto model is a tool for studying synchronization among coupled phase oscillators with a variety of applications. In the case of infinite networks of oscillators, analytic results are known for the critical coupling strength at which synchronization first occurs. Finite-sized networks pose a more difficult challenge. We propose a new interpretation of this problem using numerical algebraic geometry. This method does not depend on the coupling network or natural frequencies of the system.

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MS37

Equivariant Gröbner bases of Symmetric Toric Ideals

It has been shown previously that a large class of monomial maps equivariant under the action of an infinite symmetric group have finitely generated kernels up to the symmetric action. We prove that these symmetric toric ideals also have finite Gröbner bases up to symmetry for certain monomial orders. An algorithm is presented to compute equivariant Gröbner bases of these ideals, given the monomial map.

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MS37

Symbolic-Numeric Certification of Algebraic Sets

The topic of the talk is to use hybrid symbolic-numeric techniques to certify and enhance the handling of singularities and other degeneracies that may occur when numerically solving a system of polynomial equations. In particular, we present a new construction that completely deflates a singular root in one step. We construct a system of equations in the original variables plus a relatively small number of new variables that describes the multiplicity structure at the singular root. We show that the isolated simple solutions of this new system correspond to roots of the original system with given multiplicity structure up to a given order. This construction is exact in that it permits one to treat all conjugate roots simultaneously and can be used in certification procedures.

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MS38

A Krylov-Inspired Optimization Method for Noisy Derivatives

Many engineering systems are governed by chaotic dynamics. In general, a PDE-constrained design optimization of such chaotic systems must contend with

- large primal-space dimensions;
- expensive function evaluations, and;
- noisy data.

Together, these three characteristics challenge existing optimization algorithms. Therefore, we have developed an algorithm, using ideas from Krylov-subspace methods and statistics, that is effective at optimizing large-dimensional optimization problems in the presence of noise.

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MS38

Mathematical and Computational Challenges in High-Fidelity Aero-Thermal Design

Computational Fluid Dynamics plays an important role in industrial design and, when used appropriately, can accelerate schedules and reduce costly testing. One of the biggest challenges for industrial CFD is how to physically account for the chaotic nature of turbulence. As computers continue to grow in capability there will be a shift from approaches that model all aspects of turbulence to those that resolve certain scales for classes of problems that require higher levels of fidelity to improve accuracy. Examples of these approaches will be provided in an industrial context, successes will be shared with emphasis on accuracy, efficiency and robustness.

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MS38

Adjoint-Based Sensitivity Analysis for Large-Scale Unsteady and Chaotic Aerodynamic Simulations

Gradient-based sensitivity analysis is an enabling technology for many aerospace applications. However, conventional sensitivity analysis breaks down when applied to long-time averages of chaotic systems that may represent high-resolution simulations of turbulent aerodynamic flows. A recently proposed methodology, Least Squares Shadowing (LSS), avoids this breakdown. The first application of LSS to a chaotic flow simulated with a large-scale computational fluid dynamics solver is presented. The LSS sensitivity is accurate, but the computational cost is high.

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MS38

Chaos in High-Fidelity Simulation and Design

High fidelity simulation is a marvel of modern computational mathematics with many applications. An often ignored but important aspect of these simulations is their potential of developing chaotic dynamics. This talk shines spotlight on this aspect of high fidelity simulations. Are these simulations meaningful? How to assess if they are accurate? How to choose numerical methods and computational mesh for these simulations?

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MS39

The Method of Polarized Traces for the Helmholtz Equation

I will review the method of polarized traces, which has helped us attain sublinear runtime scalings for high-frequency Helmholtz in 2D and in 3D. Recent progress includes a HDG variant for seamless p refinement – something that was not automatic in the original framework.

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MS39

Direct Scattering by Penetrable Media

We introduce two fast algorithms for computing volume potentials - that is, the convolution of a translation invariant, free-space Green's function with a compactly supported source distribution. First, we present a new FFT-based method that can be applied in the case of uniform grids. The algorithm relies on regularizing the Fourier transform of the Green's function by cutting off the interaction in physical space beyond the domain of interest. This permits the straightforward application of trapezoidal quadrature and the standard FFT, with superalgebraic convergence for smooth data. For non-uniform grids, we use a fast direct solver which relies on the development of an automatically adaptive, high-order accurate discretization using a quad tree data structure. We have designed the algorithm to provide rapid access to arbitrary elements of the discretized system matrix. This permits the straightforward application of state-of-the-art algorithms for constructing compressed versions of the solution operator. These solvers typically require $O(N^{3/2})$ work, where N denotes the number of degrees of freedom. We demonstrate the performance of the methods for a variety of problems in both the low and high frequency regimes.

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MS39

A Multi-modes Monte Carlo Method for Wave Scattering in Random Media

In this talk, we will develop and analyze an efficient numerical method for solving the acoustic wave scattering problem in random media. The method is based upon a multi-modes representation of the solution and the Monte Carlo technique for sampling the probability space. The interior penalty discontinuous Galerkin method is applied to approximate the mode function at each sample. One key feature of the proposed numerical method is that the governing equations for all the expanded mode functions share the same deterministic Helmholtz operator. Hence an efficient direct solver by repeated use of the LU decomposition matrices can be employed, and the computational cost can be significantly reduces as a result. Error estimates of the proposed method will be discussed and the numerical experiments will be demonstrated to test the efficiency of the algorithm and validate the theoretical results.

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MS39

Fast Huygens Sweeping Method for Helmholtz Equation in High Frequency Regime

We present an efficient fast Huygens sweeping method for numerically solving the Helmholtz equation in the high frequency regime. The Huygens-Kirchhoff integral is used to integrate locally valid waves to obtain globally valid waves, where the Green's functions are approximated via the geometrical optics approximation or Babich's expansion. Asymptotic ingredients for approximating the Green's functions are computed efficiently on a coarse mesh, compressed and saved on a hard drive. Given any frequency, the asymptotic ingredients are loaded and recovered on a refined mesh where the waves are constructed by evaluating the Huygens-Kirchhoff integral by a fast multilevel butterfly algorithm. A fixed number of points per wavelength are used to construct the waves. Numerical examples are presented to verify the effectiveness of the method.

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MS40

Classical Density Functional Theory of Electrolyte Solutions

Classical density functional theory (DFT) is a statistical mechanical theory for inhomogeneous fluids, based on the minimization of a nonlocal free energy functional. I will give an overview of DFT, with particular emphasis on electrolyte solutions. I will illustrate the differences between DFT and the standard Poisson-Boltzmann theory for macroion interactions in electrolyte solutions. I will also discuss the extension of DFT to steady-state diffusion problems, and how it compares to Poisson-Nernst-Planck (PNP) theory.

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MS40

Nonlocal Modeling and Computations for Diffusion and Mechanics

We use the canonical examples of fractional Laplacian and peridynamics equations to discuss their use as models for nonlocal diffusion and mechanics, respectively, via integral equations with singular kernels. We then proceed to discuss theories for the analysis and numerical analysis of the models considered, relying on a nonlocal vector calculus to define weak formulations in function space settings. In particular, we discuss the recently developed asymptotically compatible families of discretization schemes. Brief forays into examples and extensions are made, including obstacle problems and wave problems.

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MS40

Adding More Realistic Solvent Structure to Nonlocal Electrostatics

We discuss the use of Landau-Ginzburg theory to add more realistic solvent structure to the simple Lorentz model of nonlocal dielectrics. We obtain two models that couple polarization and density fluctuations and reproduce the dielectric overscreening (charge layering) observed in experiments and atomistic simulations. Length-scale dependent coupling explains the model parameters more reasonably. Reformulating these models leads to systems of coupled local PDEs, which we solve using spectral methods. Calculations on charged parallel plates reveal surprisingly different solvent charge distributions.

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MS40

Non-Local Approximations of Boundary Value Problems

We describe an approximation of a classical diffusion operator by an integral equation with volume constraints. A particular focus is on classical diffusion problems associated with the Robin and Dirichlet boundary conditions. We explain the role of volumetric constraints as approximations to the classical boundary conditions in the presence of physical boundary and study the accuracy of such approximations.

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MS41

A Closed-Loop Context Aware Data Acquisition and Resource Allocation Framework for Dynamic

Data Driven Applications Systems (DDDAS) on the Cloud

In various DDDAS systems the sampling rates of a subset of sensors may change quickly due to changes in the execution environment, creating significant load imbalance on back-end servers, leading toward performance degradation. To address this, we investigate a closed-loop proactive resource allocation framework that adaptively reallocates resources in response to changed sampling rates. Extensive evaluation on cloud platform shows that our approach can minimize data loss significantly.

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MS41

Proper Symplectic Decomposition for Model Reduction of Forced and Dissipative Hamiltonian Systems

Recently, the proper symplectic decomposition (PSD) has been proposed for model reduction of large-scale Hamiltonian systems while preserving the symplectic structure [SIAM J. Sci. Comput., 38 (2016), pp. A1A27]. In this talk, we reformulate the dAlemberts principle to Hamiltonian form, and extend PSD for model reduction of forced and dissipative Hamiltonian systems. As an empirical approach, PSD preserves dissipativity and stability, thus, PSD is better suited than the classical POD for model reduction of hyperbolic PDEs.

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MS41

A Non-Parametric Framework for Inference Using Dynamically Deformed and Targeted Manifolds

Identifying a compact manifold on which the local solution of a nonlinear, possibly chaotic, dynamical system lies can solve many problems including inference, uncertainty quantification and model reduction. The manifold serves as a reduced model, it can be used in Bayesian inference, and enable effective re-sampling for propagating uncertainty. In this talk, we used randomized algorithms to identify the manifold produced from snapshots or initial perturbations, and show that a diffeomorphic realignment of this manifold in the presence of observations is effective in a Bayesian inference procedure and offers improvements over mixture and kernel-based methods for non-Gaussian inference. We then discuss a targeted re-sampling on the manifold to further propagate uncertainty. Examples from chaotic and nonlinear dynamical systems suggests that this approach is promising for solving the inference problems entailed by the feedback loops in DDDAS.

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MS41

Dynamic Data-Driven Decisions for Real-Time Adaptive Aircraft Path Planning

We consider path planning for an unmanned aerial vehicle that uses dynamic data-driven flight capability estimation. We propose a general approach that leverages offline analysis data and onboard sensor measurements. Formulation as a Constrained Partially Observable Markov Decision Process accounts for vehicle capability constraints and is robust to modeling error and disturbances. Sensor measurements can include combinations of multiple modalities such as GPS/IMU data as well as structural strain data of the airframe.

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MS42

Finding Reliable Communities in Complex Networks

Community detection is a widely studied problem in network analysis. However, many community detection algorithms focus on finding the best possible community and therefore can end up finding communities even in grid-like networks that do not have any community. I will talk about our recent work on developing a vertex-based community score called permanence that can quantify whether the network indeed has communities and find strong communities when they occur. I will show how permanence can be applied to non-overlapping and overlapping communities and is useful in measuring the effect of noise in disrupting the communities.

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MS42

A Combinatorially-Interpretable Matrix Factorization for Network Community Structure Evaluation

Real-world networks exhibit significant community structure. Communities are sometimes explicitly known or defined (e.g., virtual groups that one joins in an online social network, departments in an organization), but are often determined using a community detection or a clustering algorithm. Given a weighted network, with edge weights denoting interaction strengths between vertices, and a mapping of vertices to overlapping or non-overlapping communities, we present a new unsupervised method for a global community ranking, such that the computed nonnegative community weights seek to explain the edge weights. Our method is based on a new factorization of the weighted adjacency matrix. Unlike Non-negative Matrix Factorization, our decomposition has a simple combinatorial interpretation. We show that the proposed ranking problem reduces to a Non-negative Least Squares problem, and design a fast algorithm for computing the ranking. We assess this ranking problem formulation on a variety of synthetic and real-world networks, in order to gain insight into its advantages and limitations.

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MS42

Understanding Data Graphs and Their Uses

Networks and communities have been a subject of interest for decades and there are classic examples that everyone uses – citation networks, the karate club, Internet traffic, etc. Graph theory provides a mathematical framework that can represent the knowledge of such connections, but is it the best choice for the types of questions we want to answer with this data? In this talk, we will discuss the challenges inherent in turning literary descriptions into mathematical formalisms.

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MS42

Mining Citation Networks in the Scholarly Literature

Abstract Not Available at Time of Publication

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MS43

Solving Differential Equations Using Chebyshev Inner Products

We develop solutions to $\mathcal{L}u = f$ using an expansion of $u(x)$ in a Chebyshev basis, yielding a system of n equations in m unknowns which are solved using the normal equations and the discrete orthogonality relations associated with evaluating the system at the Chebyshev nodes. The boundary conditions are applied after the solution of the linear system is obtained to mitigate issues that arise due to the global nature of the solution. The method achieves superconvergence, and can be pushed to yield an order of operations approaching $O(n\, log(n))$.

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MS43

High-Order Time-Stepping for Nonlinear PDEs Through Componentwise Approximation of Matrix Functions

Krylov subspace spectral (KSS) methods are high-order accurate, explicit time-stepping methods with stability characteristic of implicit methods. This "best-of-both-worlds" compromise is achieved by computing each Fourier coefficient of the solution using an individualized approximation, based on techniques from "matrices, moments and quadrature" for computing bilinear forms involving matrix functions. In this talk, it will be shown how this approach can be applied to nonlinear PDEs.

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MS43

Numerical Simulation of Turing Pattern Formation by Edge-Based Smoothed Radial Point Interpolation Method (ES-RPIM)

We propose a robust numerical formulation for simulating pattern formation of some nonlinear reaction-diffusion Turing models in fixed 2D domains. The edge-based smoothed radial point interpolation method (ES-RPIM) is employed for spatial variations and a modified Euler method is used as the time-stepping scheme. The nonlinear terms are linearized iteratively. This procedure is based on triangular background meshes which are easy generate. The weakened weak (W2) formulation makes it possible to select locally support nodes freely for the construction of RPIM shape functions, without worrying about the compatibility issues (which we do in the standard weak formulation). The use of multiquadric (MQ) radial basis in creating RPIM shape functions ensures the non-singularity of moment matrix. We apply this method to solve the Brusselator model and simulate the pattern formation of Schnakenberg model. Since we can use as many support nodes as we like in a support domain, this method is suitable for solving Turing systems with deformed meshes. The robustness and effectiveness of this method are verified by comparing with finite element method (FEM) on deformed background meshes.

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MS43

A Localized Radial Basis Function Method for Solving Diffusion Equations

In this presentation, we introduce the Houbolt method to solve time dependent PDEs. The spatial variables are discretized by using polynomial basis and particular solutions derived from polyharmonic splines. The completeness of the selected solution basis is shown. The method discretizes the problems on the given nodes in the overlapping local domains. This feature drastically reduces the computational cost. Thus, this methods can be used to solve many types of complicated large-scale systems. The efficiency and accuracy of this particular radial basis function collocation method are validated through numerical experiments.

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MS44

Efficient Algorithms for the Simulation of Wave Propagation in Periodic Media

We presents a simple and highly efficient algorithm for evaluation of quasi-periodic Green functions that is seamlessly incorporated into a boundary integral equation numerical method for the solution of wave scattering problems by bi-periodic arrays of scatterers in three-dimensional space. Except at certain "Wood frequencies' at which the quasi-periodic Green function ceases to exist, the proposed approach, which is based on use of smooth windowing functions, gives rise to lattice sums which converge to the Green function superalgebraically fast—that is, faster than any power of the number of terms used—in sharp contrast with the extremely slow convergence exhibited by the corresponding sums in absence of smooth windowing. We establish rigorously the superalgebraic convergence of the windowed lattice sums; a variety of numerical results, in turn, demonstrate the practical efficiency of the proposed approach.

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MS44

The Windowed Green Function Method

We present a new Windowed Green Function (WGF) method for the numerical integral-equation solution of problems of electromagnetic scattering by bounded and unbounded obstacles. The approach enables solution of classical problems in the field of electromagnetic scattering, including problems of scattering by rough surfaces at Wood frequencies, problems of scattering in presence of layered dielectric media, and solution of challenging problems of transmission through junctions of open dielectric waveguides, amongst others.

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MS44

Simulation of Dispersive Effects in Dielectric-Metal Structures in the Time Domain

Abstract Not Available at Time of Publication

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MS44

A High-Order Perturbation of Surfaces/Asymptotic Waveform Evaluation (HOPS/AWE) Method for Two-Dimensional Grating Scattering Problems

The scattering of electromagnetic waves by periodic gratings is important in applications. High-Order Perturbation of Surfaces (HOPS) methods were devised by Milder and Bruno & Reitich for the rapid and robust simulation of these interactions. With a single simulation, for fixed illumination frequency, these methods produce returns for an arbitrary selection of grating heights. We describe a novel HOPS/Asymptotic Waveform Evaluation algorithm which, with a single computation, generate simulations for arbitrary depth and frequency granularity.

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MS45

Superconvergent Hdg Methods for Third-Order Linear Equations in One-Space Dimension

We design and analyze the first hybridizable discontinuous Galerkin methods for third-order linear equations in one-space dimension. The methods are defined as discrete versions of characterizations of the exact solution in terms of local problems and transmission conditions. They provide approximations to the exact solution u and its derivatives $q := u'$ and $p := u'$ which are piecewise-polynomials of degree k_u, k_q and k_p, respectively. We consider the methods for which the difference between these polynomial degrees is at most two. We prove that all these methods have superconvergence properties which allows us to prove that their numerical traces converge at the nodes of the partition with order at least $2k + 1$, where k is the minimum of k_u, k_q, k_p. This allows us to use an element-by-element post-processing to obtain new approximations for u, q and p converging with order at least $2k + 1$ uniformly. Numerical results validating our error estimates are displayed.

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MS45

Adaptive HDG Schemes on Near-Optimal Meshes

We present an anisotropic mesh adaptation and optimization method for hybridizable discontinuous Galerkin (HDG) Schemes. Given the total number of dofs, we propose a metric-based method, which aims to globally minimize the L^q norm of an error model associated with the approximation space. Defining a suitable continuous interpolation operator allows us to use an analytic optimization framework, which operates on the metric field, rather than the discrete mesh. We present numerical validation for convection-diffusion systems.

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MS45

Analysis of the HDG Method for the Stokes-Darcy Coupling

In this talk we introduce and analyze a hybridizable discontinuous Galerkin (HDG) method for numerically solving the coupling of fluid flow with porous media flow. Flows are governed by the Stokes and Darcy equations, respectively, and the corresponding transmission conditions are given by mass conservation, balance of normal forces, and the Beavers-Joseph-Saffman law. We consider a fully-mixed formulation in which the main unknowns in the fluid are given by the stress, the vorticity, the velocity, and the trace of the velocity, whereas the velocity, the pressure, and the trace of the pressure are the unknowns in the porous medium. In addition, a suitable enrichment of the finite dimensional subspace for the stress yields optimally convergent approximations for all unknowns, as well as a superconvergent approximation of the trace variables. To do that, similarly as in previous papers dealing with development of the *a priori* error estimates, we use the projection-based error analysis in order to simplify the corresponding study. Finally, we provide several numerical results illustrating the good performance of the proposed scheme and confirming the optimal order of convergence provided by the HDG approximation.

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MS45

HDG Methods for Nonlinear Elasticity

We revisit the HDG methods for nonlinear elasticity problems studied in SC. Soon (2008) and Kabaria, et al. (2015). In particular, we first propose a local post-processing for the standard HDG methods. Numerical results suggest that our HDG methods is super-convergent. On the other hand, we conduct a stability analysis on the example proposed by Kabaria, et al. (2015), where numerical experiment displayed non-convergent results when the stabilization function $\tau = 1$ on all faces. Our analysis deduce a new stabilization strategy for HDG methods. Numerical experiment in 2D support that our new strategy can ensure stability of HDG methods without sacrificing optimal convergence. Finally, we propose several implementation modifications based on a discrete minimization principle, with which we can further improve the efficiency of HDG methods.

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MS46

Active Subspaces for Dimension Reduction in Parameter Studies

Active subspaces are part of an emerging set of tools for reducing the dimension of a complex simulation model's input parameter space. One must first discover a model's active subspace by studying the gradient of a quantity of interest with respect to the inputs. If a model shows evidence of an active subspace, then techniques exist to exploit the low-dimensional structure for computations that suffer from the curse of dimensionality, such as constructing response surfaces.

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MS46

Asymptotically Exact MCMC Using Local Approximations in Likelihood-Informed Subspaces

Abstract Not Available at Time of Publication

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MS46

Reduced Basis Anova Methods for Partial Differential Equations with High-Dimensional Random Inputs

We present a reduced basis ANOVA approach for partial deferential equations (PDEs) with random inputs. The ANOVA method combined with stochastic collocation methods provide model reduction in high-dimensional parameter space through decomposing high-dimensional inputs into unions of low-dimensional inputs. In this work, to further reduce the computational cost, we investigate spatial low-rank structures in the ANOVA-collocation method, and develop efficient spatial model reduction techniques using hierarchically generated reduced bases. We present a general mathematical framework of the methodology, validate its accuracy and demonstrate its efficiency with numerical experiments.

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MS46

Stochastic Collocation with Multi-Fidelity Models

We shall discuss a numerical approach for the stochastic collocation method with multifidelity simulation models. The method combines the computational efficiency of low-fidelity models with the high accuracy of high-fidelity models. We shall illustrate the advantages of the method via a set of more comprehensive benchmark examples including several two-dimensional stochastic PDEs with high-dimensional random parameters. Finally, We suggest that tri-fidelity simulations with a low-fidelity, a medium-fidelity, and a high-fidelity model would be sufficient for most practical problems.

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MS47

A Structured Two-Stage Population Model with Migration

A structured population is one with consistent differences among the members of the population. Here, we partition the population by reproductive maturity. We take two such populations of the same species in adjacent locations and consider migration between the two locations. When constant breeding and migration are considered, we propose simple conditions under which the model has a unique globally attracting periodic state. These conditions are simpler than those given by other authors. We apply our theory to a generalized version of the model with a larger number of patches and a periodically varying environment and under different, but still simple, conditions reach the same conclusion.

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MS47

Statistical Text Analysis of Guyanese Suicide-related News Data

According to World Health Organization (WHO), the small South American country of Guyana has the highest rate of suicide in the world. Furthermore, it is hypothesized that suicide can be prevented, provided identification of people at risk and early intervention. This talk investigates the application of text analysis techniques to suicide-related news data, specifically newspapers, magazines, and websites. We show how automatically extracted relevant event data from available electronic text collections reveals interesting patterns of geographic, demographic, and other social factors in communities affected by suicide. We seek to not only illustrate the utility of applying text mining techniques to this important public health issue, but leverage how these computational, linguistic, and statistical methods can provide valuable indicators underlying this phenomena.

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MS47

Discussion on a "Possible" Biological Application of Knot Floer Homology

The study of DNA knots and links are of great interest to molecular biologists as they are present in many cellular processes. The variety of experimentally observed DNA knots and links makes separating and categorizing these molecules a critical issue. This discussion focuses on reviewing methods for finding the knot Floer homology for two biologically relevant subfamilies: $(2, p)$-torus knots and (q, r, s)-pretzel knots and the a possible application for these invariants.

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MS47

Optimal Scheduling of Antiangiogenic and Chemotherapeutic Cancer Treatments

Anti-angiogenic drugs – drugs that restrict the creation of new blood vesselshave recently become of particular interest as an avenue of cancer treatment. We have developed a non-linear, mixed-effect ODE model as a strategy to quantify the dynamics of tumor growth, vasculature generation, chemotherapy, and anti-angiogenic treatment. This model accurately predicts tumor growth dynamics of colorectal tumor growth data and allows us to predict optimal treatment schedules of combined anti-angiogenic and chemotherapeutic treatment.

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MS48

Analysis of the Open Pit Mining Problem from a Shape Optimization Perspective

The present work gives the variational tools to begin the analysis of the Ultimate Pit Limit Problem, which arises in open pit mining. A recent formalization developed by Juan Ignacio Guzman allowed to understand this problem from a mathematical point of view, exposing the related shape optimization problem. With this, we took the most basic structure present in the problem and analysed it to verify that the problem is well-posed. Many of the challenges appearing in this kind of problems are inherent to all shape optimization problems, such as the difficulty to define a comfortable topology in the admissible deformations space or the numerical implementation. For this objective, we present a simple variational approach and show that it is indeed equivalent to the shape optimization problem. We end with various examples to show how each approach behaves, together with a solution given by the classical Lersch & Grossman method to see how they compare.

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MS48

Internal Numerical Differentiation Approach for Parameter Estimation for Two-Dimensional Partial Differential Equation Problems

The numerical solution of the parameter estimation problem constrained by a Partial Differential Equation is considered. For the evaluation of the derivatives tailored methods of Internal Numerical Differentiation of the Partial Differential Equation solution are developed. Algorithmic Differentiation is applied to a part of the discretized Partial Differential Equation and the structure is exploited to reduce the numerical costs. Future objectives include optimum experimental design of chemical experiments, where higher derivatives need to be evaluated.

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MS48

Modeling Self-Shading of Light on Kelp Growth in Aquaculture Operations

Understanding the growth rate and nutrient absorption of kelp cultures has important marine biological implications. Current models for kelp growth place little emphasis on the way in which nearby plants shade one another. Self-shading may be a significant model feature, though, as light availability may impact the growth and composition of the kelp biomass. We seek to use differential equations among other modeling techniques to more accurately describe this aspect of kelp growth.

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MS48

Pediatric ECG Feature Identification

Since each part of the electrocardiogram (ECG) corresponds to a different stage in the cardiac cycle, automatically tracking changes in individual ECG features over time can help physicians gain insight into a patient's clinical status. Existing algorithms, however, are not typically designed for pediatric populations. To meet this need, we are using the CUR matrix factorization and statistical learning methods to identify ECG features, working toward the development of predictive models for clinical decision support.

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MS48

Generating Audio Mixtures Using Deep Convolutional Neural Networks

Deep neural networks have recently been used in a generative capacity to separate and convolve the content and style of two input images. This is done using a joint cost function during gradient descent that encodes information about style and content to iteratively calculate forward node activations. We extend this methodology to the auditory domain using sound clips converted to spectrograms using the short-time Fourier transform and discuss optimizing signal reconstruction.

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MS48

A Second Order Time Homogenized Model for Sediment Transport

A multi-scale method for the hyperbolic systems governing sediment transport in subcritical case is developed. We first derive a zeroth order homogenized model, and then propose a first order correction. We develop a second order numerical scheme following the framework of heterogeneous multi-scale method. The numerical results in both one and two dimensional cases demonstrate the effectiveness and efficiency of our method.

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MS49

Solving Inverse Modeling in Subsurface Hydrology Using a Computationally Efficient Levenberg-Marquardt Algorithm

Inverse modeling seeks transitivity field given measurements of hydraulic heads. However, practical problems are often large scale, and conventional methods can be computationally expensive. We have developed a new, computationally-efficient Levenberg-Marquardt method for solving large-scale inverse modeling problems. Our method is based on a recycled-Krylov subspace technique. We apply our method to invert for a random transitivity field and obtain a significant speedup. Therefore, our new inversion method is a powerful tool for large-scale applications.

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MS49

Optimization via Parametric Model Reduction with Stochastic Error Estimates

While parametric model reduction offers significant computational savings for evaluation heavy applications, such as parameter inversion and optimization, its use is tempered by concerns for the approximation error. For reduced order models with many parameters, error bounds are typically not available or only at a very high cost. In this work, we will explore inexpensive stochastic estimates for the approximation error and how these estimates can be used to guide the optimization process and update the reduced order model.

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MS49

Inner-Outer Krylov Methods for Diffuse Optical

Tomographic Image Reconstruction

Recovering an absorption image in diffuse optical tomography requires the solution of a sequence of large-scale, shifted linear systems with multiple right-hand sides. While reduced order models can be used to replace the large-scale systems, they must still be computed. An inner-outer Krylov recycling method was recently developed by O'Connell, et. al for the non-shifted case to reduce this cost. In this talk, we extend this approach to the shifted case.

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MS49

Reduced Order Modeling in Photoacoustic Tomography

Photoacoustic tomography combines a rich optical contrast with the high resolution of ultrasound tomography. Mathematically it is an ill-posed inverse coefficient problem for a coupled wave equation and diffusion equation pair. Since the wave speed is assumed to be constant, to accelerate the inversion, we use a Hessian-based reduced order model for the wave equation. We demonstrate the computational gains on a synthetic problem motivated from neuroscience.

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MS50

Subsurface Flow Model Calibration Under Uncertain Geologic Scenarios

In calibration of subsurface flow model, the conceptual geologic connectivity scenario (e.g., a variogram) is treated as a constraint. We develop a group-sparsity formulation to use the flow data to discriminate against multiple proposed geologic scenarios. During model calibration, the group-selection property of the formulation is exploited to search over alternative geologic dictionaries to eliminate those that are not supported by the data while constructing a calibrated model using components from the consistent scenario(s)

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MS50

A Surrogate Accelerated Multicanonical Monte Carlo Method for Uncertainty Quantification

In this work we consider a class of uncertainty quantification problems where the system performance or reliability is characterized by a scalar parameter y. The performance parameter y is random due to the presence of various sources of uncertainty in the system, and our goal is to estimate the probability density function (PDF) of y. We propose to use the multicanonical Monte Carlo (MMC) method, a special type of adaptive importance sampling algorithm, to compute the PDF of interest. Moreover, we develop an adaptive algorithm to construct local Gaussian process surrogates to further accelerate the MMC iterations. With numerical examples we demonstrate that the proposed method can achieve several orders of magnitudes of speedup over the standard Monte Carlo method.

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MS50

Fast Deployment of Surrogate Modelling-Based Uncertainty Quantification Techniques Using UQLab

Surrogate models are becoming ubiquitous in many fields of uncertainty quantification. They enable the use of advanced UQ techniques (e.g. Monte-Carlo simulation, reliability-based design optimization, structural reliability, sensitivity analysis) even in the presence of the costly computational models used in complex manufacturing environments. In this contribution we give an overview of how the UQLab software framework can be used to rapidly deploy complex surrogate-modelling based techniques to solve various types of industrial UQ problems.

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MS50

Multifidelity Reliability Analysis

Abstract Not Available at Time of Publication

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MS51

Heuristic Methods for Choosing Paths In Homotopy Methods

The core method to Numerical Algebraic Geometry is Homotopy Continuation. This method is robust, but fails at singularities. These singularities can cause the method of Homotopy Continuation to slow if we are near their location. In this talk we discuss methods for avoiding such singularities and the problems they cause.

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MS51

Numerical Algebraic Geometry and Multiparameter Equations of State

Multiparameter equations of state arise in thermodynamics to describe the changes in matter states under given temperatures and pressures. These typically polynomial-exponential equations depend on parameters which are only known approximately. The behavior of these equations near critical temperatures is of most interest, but ill-conditioning encumbers traditional numerical approaches. We present a method using numerical algebraic geometry to compute this behavior near these critical temperatures and apply this method to a variety of fluids.

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MS51

Numerical Algebraic Geometry for Exploring Systems Biology Models

Abstract Not Available at Time of Publication

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MS51

Understanding Quantum Adiabatic Computing via Numerical Algebraic Geometry

Quantum Adiabatic Computing (QAC) is perhaps the most common model used in quantum computation. This model relies on the so-called Adiabatic Theorem initially observed by scientists in the early 20th century. Roughly speaking, this theorem states that if a Hamiltonian system is perturbed slowly, then the associated energy states of the system also change slowly. This theorem is the foundation of QAC. In this talk, I will provide a brief overview QAC and its relation to both Numerical Algebraic Geometry and Random Matrix Theory, some challenges associated with the model, and potential solutions. This is joint work with Xun Gao and Lei Zhixian from The Institute for Interdisciplinary Information Sciences at Tsinghua University.

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MS53

Non-Intrusive Lease Square Shadowing Sensitivity Analysis via Projection

In engineering it is crucial to carry out sensitivity analysis on the nonlinear system, which often bear chaotic motion even with relatively low-fidelity simulation. However, this sensitivity analysis always breaks down with traditional methods. The Least Squares Shadowing (LSS) has been developed in order to redefine a numerically feasible sensitivity problem with rigorous theoretical foundation. This paper develops a new variant of the LSS method, which has successfully computed the derivative for several chaotic ODEs and PDEs. The development in this paper aims to make the LSS method a non-intrusive method and reduce the time and memory cost, by using the idea of projection when solving the LSS problem. Instead of constructing a big matrix and do an inverse, this new variant first calculate the inhomogeneous version of the constraint problem, then subtract from it its projection on the function space spanned by the homogeneous solution of the constraint problem. This new variant could make LSS faster and easier to use when dealing with engineering problems.

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MS53

Output Error Estimation for Chaotic Systems

Due to the butterfly effect, adjoint-based error estimation has proven to be more difficult to implement for chaotic flows. We show one promising solution that appeals to statistical averages of the output error over short time windows. These shorter windows yield statistically useful error information before the chaotic system exponentially changes. We demonstrate the method for prototypical

chaotic systems, including the modified one-dimensional Kuramoto-Sivashinsky equation.

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MS53

Stabilized Unsteady Adjoint of Large Eddy Simulations

An unsteady adjoint of large eddy simulations is useful for design optimization. But the method provides diverging gradients for long time-averaged objectives due to chaotic dynamics of turbulence. An energy analysis of the compressible Navier-Stokes adjoint equations suggests that adding artificial viscosity to the adjoint equations can limit it's divergence and maintain accuracy of sensitivities. Results for chaotic flow over a cylinder and turbine vane will be presented.

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MS54

Accurate and Efficient Nystrom Volume Integral Equation Method for the Maxwell Equations for 3-D Scatterers

In this talk, we present an accurate and efficient Nystrom volume integral equation (VIE) method for the Maxwell equations for a large number of 3-D scatterers. The Cauchy Principal Values that arise from the VIE are computed accurately using a finite size exclusion volume together with explicit correction integrals consisting of removable singularities. Also, the hyper-singular integrals are computed using interpolated quadrature formulae with tensor-product quadrature nodes for cubes, spheres and cylinders, that are frequently encountered in the design of meta-materials. The resulting Nystrom VIE method is shown to have high accuracy with a small number of collocation points and demonstrates p-convergence for computing the electromagnetic scattering of these objects. Numerical calculations of multiple scatterers of cubic and spherical shapes validate the efficiency and accuracy of the proposed method.

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MS54

Computation of Electromagnetic Fields Due to a Dipole Source in Multilayered Media

In this talk, computation of electromagnetic waves due to a dipole source located in multilayered media will be presented. Both electric and magnetic fields are expressed in the spectral domain. Then, all the correction terms from layer interfaces are computed with generalized reflection and transmission coefficients. Then, Sommerfeld integrals are taken to recover the fields in physical domain. By construction, all the correction terms have no singularities. As a result, most numerical methods developed for the free-space can be easily applied to the multilayered media.

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MS54

Second Kind Integral Equation Formulation for Mode Calculation of Optical Waveguides

In this talk, we present a second kind integral equation (SKIE) formulation for calculating the electromagnetic modes of optical waveguides, where the unknowns are only on material interfaces. The resulting numerical algorithm can handle optical waveguides with a large number of inclusions of arbitrary irregular cross section, including non-smooth geometries. Our method is highly accurate and thus can be used to calculate the propagation loss of the electromagnetic modes accurately, which provides a reliable numerical tool for the design of more compact and efficient photonic devices, as well as the inverse problem to reconstruct the dielectric constant of the optic fibers.

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MS54

Fundamental Limits to Wave Scattering in Linear Media

Are there limits to the power that can be absorbed/scattered/radiated by an arbitrary scattering body? By virtue of an integral-equation formulation of the optical theorem, I use energy-conservation principles to demonstrate such scattering bounds for lossy media (e.g. metals at optical frequencies), at any frequency and independent of bandwidth, that depend only on the intrinsic material parameters of the structure. The energy-conservation approach can be extended to the problem of near-field radiative heat transfer, with stochastic sources inside one of the bodies, via two scattering problems connected by reciprocity. By connecting the energy-conservation approach to the stored energy in any optical resonance, power–bandwidth limits for a single resonance can be derived for any material, lossy or lossless. I briefly present scenarios in which known structures can reach these bounds, and also scenarios in which all known structures fall far short, suggesting areas where new design may result in dramatic performance improvements.

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MS55

Multiscale Schwarz Coupling for Capturing Boundary Effects in Dilute Charged Particle Systems

It is well–known that the memory requirements to solve nonlocal equations are prohibitive for large domains and fine meshes. In the classical density functional theory (cDFT) model, the nonlocal effects of the density distribution occur in some small finite neighborhood of a surface in the fluid domain. Outside this neighborhood, the nonlocal effects diminishes and a local description is sufficient to model the drift– diffusion behavior of the charged particle system. In this work, we present results from utilizing the Schwarz alternating procedure to couple cDFT to the PNP equations for determining the behavior of charged particle systems in larger domains.

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MS55

Collocation Method for One Dimensional Nonlocal Diffusion Equations

In this paper, collocation method for solving one dimensional steady state and time dependent nonlocal diffusion equations is analyzed. The difficulty of applying collocation method to nonlocal diffusion equations comes from the singularity of the kernel. If $s < \frac{1}{2}$ it is weakly singular integral, however, if $s \geq \frac{1}{2}$ the integral is not integrable in Riemann sense. So that the Hadamard finite part integral is introduced to overcome this difficulty. But new things bring new troubles. For analysis and performance, a "balance" term is added to discretize the nonlocal operator. Numerical results verify the theorems.

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MS55

Simulation of Nonlocal Electrostatics in Python Using Fenics and Bem++

Abstract Not Available at Time of Publication

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MS55

Finite Element Approximations of Nonlocal Electrostatics Models

In this talk, we present preliminary results on the finite element discretization of nonlocal electrostatic models given by integro-differential equations. Numerical experiments will be presented to support theoretical results. This work is in collaboration with Nathan Baker and Alexandre Tartakovsky.

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MS56

Data-Driven Optimal Learning for Dynamic Online Flight Capability Estimation for Self-Aware Aerospace Vehicles

A self-aware aerospace vehicle can dynamically adapt the way it performs missions by gathering information about itself and its surroundings and responding intelligently. We present an information-theoretic approach to offline learning via the optimization of libraries of strain, capability, and maneuver loading using physics-based computational models. Online capability estimation is then achieved using by a Bayesian classification process that fuses dynamic, sensed data.

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MS56

Dynamic Data-Driven Modeling of Multi-Stage Nanocrystal Growth Using in-Situ Tem Video Data

This work presents a dynamic, data driven method for detecting the phase change points in a nanocrystal growth trajectory using in-situ TEM video data. Such methods are pressingly needed, as the in-situ TEM technique is used more and more routinely nowadays, producing motion picture data at a rate beyond manual processing capability. Detecting change points produce strong clues about where to explore for understanding the basic science behind the highly stochastic nanocrystal self-assembly processes.

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MS56

Real-Time Vehicle Detection and Tracking Dddas Using Hyperspectral Features from Aerial Video

Vehicle detection from a moving aerial platform poses a number of unique challenges. In this talk, we consider a DDDAS framework for controlling an adaptive multimodal sensor to design a real-time detection system. Wide field of view (FOV) panchromatic imagery is used to remove global camera motion and adaptively chosen narrow FOV hyperspectral data is considered to detect the target of interest (TOI). The system is evaluated in a synthetic, realistic, and dense scene.

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MS56

Reduced-Space Gaussian Process Regression Forecast for Nonlinear Dynamical Systems

We consider the problem of short term prediction of high-dimensional chaotic dynamical systems possessing lower-dimensional attractors. We formulate a data-driven stochastic dynamical model in a reduced order subspace, which consists i) of a data-driven mean vector field, and ii) a zero-mean stochastic component that captures the uncertainty induced by the un-modeled coordinates. The stochastic model is estimated using a spatially Gaussian process regression. Applications are presented for the Lorenz 96 system and other chaotic systems.

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MS57

Physical and Mathematical Modeling of Chemical Enhanced Oil Recovery

Enhanced oil recovery techniques involve multi-phase multi-component multi-physics flows of complex fluids using a variety of flooding schemes. Fluid dynamics of these complex fluids through porous media which takes into all possible effects present in such flows are poorly understood and are difficult to model accurately, We will discuss various issues involved in accurate physical modeling and discuss development of modern numerical methods to solve complex systems of PDEs in these models.

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MS57

Numerical Analysis of a Hybrid Method and Large Scale Simulation Results of SP-Flooding

We propose a two-phase porous media flow model for surfactant-polymer flooding which incorporates the capillarity effect and also the effect of polymer and surfactant on viscosity, interfacial tension and relative permeabilities. We define a new global pressure and solve the coupled system of equations using a new hybrid method. We discuss the convergence analysis. Numerical simulations qualitatively validate the method and help to evaluate the relative performance of various flooding schemes for several heterogeneous reservoirs.

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MS57

Forward and inverse problems for multiphase flow through porous media

Mathematical models of fluid flow problems in porous media result in non-stationary, non-linear (system of) Partial Differential Equations (PDEs). As PDE-solvers mature, there is increasing interest in industry and academia in solving optimization problems governed by those PDEs. For these problems a sensitivity-based multiple-shooting method has been developed in which optimality is achieved simultaneously with the feasibility of the state equations. Some of the results of this method will be presented.

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MS57

Bayesian Framework for Validation of Models for Subsurface Flows

We present a new Bayesian framework for the validation of subsurface flow models. We use a compositional model to simulate CO2 injection in a core, and compare simulated to observed saturations. We first present computational experiments involving a synthetic permeability field. They show that the framework captures almost all the information about the heterogeneity of the permeability field of the core. We then apply the framework to real cores, using data measured in the laboratory.

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MS58

Relational Object Analysis Drives Multi-Modal Attack Prediction (Roadmap)

ROADMAP detects signals prior to a cyber attack, allowing prediction and warning to prevent data and monetary loss. Utilizing a layered approach, we store relevant data and relationships in a rich, yet uniformly represented, graph. The graph simplifies extraction, fusion, and prediction activities without sacrificing timeliness or accuracy. Higher layers combine cyber attack and cyber actor models with Bayesian nonparametric machine learning techniques to handle model drift, capture expert knowledge, and bootstrap learning in low-signal situations.

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MS58

Probabilistic Forecasting in the Presence of Noisy and Conflicting Evidence

Big and noisy data presents challenges to traditional forecasting techniques, limiting their specificity and accuracy. Challenges become even greater when data relevant to target events is sparse and spread across many sources. We present results from developing the *Exploiting Leading Latent Indicators in Predictive Sensor Environments* (ELLIPSE) system, which forecasts cyber attacks using scalable, probabilistic models that combine noisy and conflicting evidence from multiple sensors and incorporate background knowledge to learn from limited training data.

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MS58

Predicting Events Using Diverse Ensemble Models

Predicting events in complex systems, such as sociocultural dynamics, is notoriously difficult. We present three ensemble combinations that can mitigate the complexity of predictive modeling: (1) using a variety of analytic approaches over different data types; (2) applying different approaches to address particular aspects of the modeled system; and (3) merging the results of several parallel approaches into a single coherent analysis. We also explore various techniques for combining modeling approaches in these ensembles.

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MS58

Mathematical Challenges in Predictive Analytics

Practitioners of predictive analytics face a number of challenges. Feature data is often large and noisy. Proper ground-truth labels are often unavailable, forcing the use of proxies assembled from incomplete data collected for another purpose. There is no consensus on how to evaluate prediction quality. I will outline mathematical aspects of these challenges.

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MS59

Mapping Communities Across Graphs via Edge Cover

We present experimental results of mapping corresponding communities across networks created from MRI scans of brains, flow cytometry images of immune systems, and segmentations of temporal image sequences. A combinatorial algorithm, called the mixed edge cover (MEC), is at the heart of our approach. MEC allows a community from one graph to be matched with zero, one, or more communities in another graph. Thus, it offers more flexibility than a matching or edge cover.

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MS59

Multiscale Anomaly Detection on Time-Varying Graph Data with Cyber Applications

This talk will present developments for detecting anomalies in a sequence of graphs at multiple related levels (node, community, and full graph level). The techniques allow users to "zoom-in' on anomalies. Two techniques are presented. The first uses statistics describing node degrees and community interaction to detect abnormalities. The second counts graphlets (small, induced subgraphs) and their automorphism orbits, and performs outlier detection on the resulting sequence of vectors. Cyber-security applications will be presented.

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MS59

How Can We Learn from a Trillion-Edge Graph?

If each edge of a graph requires 24 bytes to represent it, then a trillion edges requires 24TB of memory. Data of this size precludes most analysis techniques simply by its sheer size. Very few servers can accommodate that data size without paging some of the graph out to disk, resulting in unacceptable performance. So what can we do to learn from data of this size? This talk will provide an overview of work being done at PNNL in the area of High Performance Data Analytics, which consists of applying High Performance Computing (HPC) solutions to really large data.

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MS59

Mining for Communities in Large-Scale Graphs

Community detection is a widely used graph operation aimed at discovering tightly-knit subsets of vertices from an input graph. It finds application in a number of scientific and social computing disciplines. However, implementing the operation at scale remains a daunting challenge owing to inherent irregularity coupled with the lack of parallel architectures ideally suited for graph data structures. In this talk I will present challenges and recent algorithmic advances for efficient parallel community detection.

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MS60

Residue-Error Cross Validation, a New Method On Selecting An Optimal Shape Parameter For RBF Approximation

A new method, Residue-Error Cross Validation (RECV), is developed for selecting a shape parameter which provides accurate results for Kernel-Based Collocation (KBC) meshless method utilizing Radial Basis Functions (RBFs), such as Multiquadratic, and Gaussian, contain a shape parameter. The RECV method can easily map the original optimization problem of defining a shape parameter into a root-finding problem, thus avoiding the local optimum issue associated with the resultant matrix, which is inherently ill-conditioned, and obtained the numerical result accurately.

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MS60

A Mixed Finite Element Method for a Sixth Order Elliptic Problem

We consider a mixed finite element method for a sixth order partial differential equation. The method is very close to a method due to Ciarlet and Raviart for the biharmonic equation. We prove optimal a priori estimates for our approach.

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MS60

Fast Method of Approximate Particular Solutions with Polyharmonic Splines As RBFs

Fast method of approximate particular solutions (FMAPS) is an efficient meshless method which is based on the method of approximate particular solutions (MAPS). In this work, we use Polyharmonic splines (PS) as RBFs in the FMAPS to approximate the numerical solution of the given PDEs. Numerical results confirm that FMAPS with PS is extremely accurate and efficient for the elliptic PDEs on the irregular domains.

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MS60

Method of Fundamental Solutions Using Transformed Angular Basis Functions

In this talk, we introduce transformed angular basis functions(ABFs) that can be used in the method of fundamental solutions (MFS) as basis functions. The idea of ABF was proposed by Young et al. in 2015, but its implementation was limited by the selection of source points. By the transformation we designed, the source points can be selected in a similar way to traditional MFS using radial basis functions. Numerical experiments on solving interior and exterior potential flow problems governed by the 2-D Laplace equation will be presented.

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MS61

Hybrid Numerical-Asymptotic Boundary Element Methods for High Frequency Scattering

High frequency scattering is notoriously challenging for conventional numerical methods (e.g. finite and boundary element methods). Hybrid numerical-asymptotic (HNA) methods aim to significantly reduce computational cost by enriching the numerical approximation space with oscillatory functions, carefully chosen to capture the high frequency asymptotic behaviour of the solution. I will describe recent advances in HNA boundary element methods for transmission problems (dielectric scatterers), relevant e.g. to light scattering by atmospheric ice crystals.

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MS61

High-Order Perturbation of Surfaces Methods for Electromagnetic scattering: Multi-Layered Periodic Structure

A High-Order Perturbation of Surfaces Methods for Electromagnetic scattering in a multi-Layered periodic medium. We look for an accurate numerical solution of the two dimensional Helmholtz equations in the layered periodic structure (triple layered) using High-Order Perturbation of Surfaces methods. Introducing an artificial boundaries which truncate the computational domain using Dirichlet-to-Neumann map, we reformulate the Helmholtz equations in a three layered structure and derived the governing equations. Utilizing the transformed fields expansions, accurate numerical solutions are demonstrated via modified Legendre-Galerkin methods. The numerical simulations show that the proposed algorithm obtain a spectral convergence.

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MS61

Analysis and Computation of Topologically Protected Edge States in Honeycomb Structures

Topologically protected edge states are of great current interest in condensed matter and photonic systems, such as graphene and artificial graphene. In this talk, we first outline a rigorous bifurcation theory of topologically protected edge states in such 2D honeycomb structures, in both electronic (Schrödinger) and photonic (Maxwell) settings. We then present numerical results obtained by finite difference, finite element and spectral methods, which play an important role in our investigations of edge states.

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MS61

Scalable High-Order Algorithms for Large-Scale Electromagnetic Systems

Efficient and scalable algorithms are critical to deliver numerical PDE solutions fast for important scientific applications. This talk will discuss recent development on high-order spectral-element discretizations for solving the governing PDEs for electromagnetic systems. Discussion will include the algorithmic strategies on fast operator evaluations and minimizing communication cost that are key components to achieve a fast simulation on the advanced computing platforms.

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MS62

Output-Based Mesh and Order Optimization for the Hybridized Discontinuous Galerkin Method

We present a strategy for optimizing the distribution of degrees of freedom in a high-order HDG discretization. The method is output-based and relies on the solution of an adjoint in a refined approximation space. Both mesh size (anisotropic h) and order distribution (p) are considered for adaptation mechanics, and local optimization problems dictate the most efficient resource investment. Results for the compressible Navier-Stokes equations demonstrate the robustness of the resulting adaptive method.

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MS62

An Adaptive SDG Method for Incompressible Flows

We derive a residual-type a-posteriori error estimator for the Stokes system solved with the staggered discontinuous Galerkin (SDG) method. This adaptive method is suitable for solving problems with singularities and for computing flows in perforated domains, where solutions have complex features. The SDG method is recently shown its relation to the HDG method. Thus, the method and theory developed can also be applied to HDG for the Stokes system.

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MS62

Iterative Methods for EDG and HDG

Embedded DG (EDG) and Hybridizable DG (HDG) methods are new classes of the Discontinuous Galerkin (DG) method. Compared to classical DG methods, the number of globally coupled degrees of freedom for EDG and HDG methods is significantly smaller. However, whether EDG and HDG methods are more efficient than DG methods depends for a large part on the efficiency of iterative methods for the discrete systems. This will be the topic of this talk.

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MS62

Sparse Grid Discontinuous Galerkin Schemes for High-Dimensional PDEs

In this talk, we will discuss sparse grid DG methods for computing high-dimensional PDEs. Using a hierarchical basis representation, we construct a sparse finite element approximation space, reducing the degree of freedom from the standard $O(h^{-d})$ to $O(h^{-1}|\log_2 h|^{d-1})$ for d-dimensional problems, where h is the uniform mesh size in each dimension. The accuracy of the numerical approximation of this method is only slightly deteriorated, which is verified by error estimates and numerical tests in multi-dimensions. Applications of the scheme to kinetic simulations are discussed.

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MS64

The Role of RdCVF in the Health of Cone Photoreceptors

Understanding the essential components and processes for co-existence of rods and cones is at the forefront of retinal research. The recent discovery on RdCVFs mechanism and mode of action for enhancing cone survival brings us a step closer to unraveling key questions of coexistence and co-dependence of these neurons. In this work we build from ecological and enzyme kinetic work on functional response kinetics and present a mathematical model that allows us to investigate the role of RdCVF and its contribution to glucose intake. Our model results and analysis predict a dual role of RdCVF for enhancing and repressing the healthy co-existence of the rods and cones. Our results show that maintaining RdCVF above a threshold value allows for co-existence. However, a significant increase above this value threatens the existence of rods as the cones become extremely efficient at uptaking glucose and begin to take most of it for themselves. By understanding the contributions of rods to cones survival via RdCVF in a non-diseased retina we hope to shed light on degenerative diseases such as Retinitis Pigmentosa.

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MS64

Simulations of Walking Droplets in a Harmonic Potential

We present the results of a theoretical investigation of the dynamics of droplets walking on the surface of a vibrating bath while subjected to a radial spring force. This system was first explored by Perrard et al. (2014) and Labousse et al. (2016), who reported a number of orbital states characterized by a double quantization, in mean radius and angular momentum. Particular attention is given here to characterizing the dependence of the system behavior, specifically the quantization, on the vibrational forcing and the spring force. A number of new exotic orbital states are identified.

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MS64

Mathematical Models for Bone Formation and Metabolism

Bone remodeling is an elegant and tightly regulated multicellular process by which osteocytes, osteoblasts and osteoclasts function as a syncytium to maintain or modify bone. In this work we developed a mathematical model of bone formation validated with experimental data obtained from osteoblastic bone cells induced to mineralize and quantified at 26 days of culture. A Cellular Automata model was constructed to simulate the *in vitro* experiments. Statistical methods where used to validate the model.

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MS64

Mathematical Modeling of Fungal Infection in Immune Compromised Individuals: The Effect of Back Mutation on Drug Treatment

We present a model that describes treatment of a fungal infection in an immune compromised patient in which both susceptible and resistant strains are present with a mutation allowing the susceptible strain to become resistant as well as a back mutation allowing resistant fungus to again become susceptible using nonlinear differential equations. Using bifurcation theory and sensitivity analysis, we show the model demonstrates that under any levels of the drug both strains will be in stable co-existence and high levels of treatment will never completely eradicate the susceptible strain. We discuss the model and implications for treatment options within the context of an immune compromised patient.

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MS65

An Overset Mesh Hybridizable Discontinuous Galerkin Fluid-Structure Interaction Algorithm

Coupling the hybridizable discontinuous Galerkin method with overset meshing enables solutions to complex multiphysics partial differential equations (PDEs). The focus here is a fluid-structure interaction PDE system. The overset meshes allow for efficient mesh motion to occur under large solid deformation. There are two types of overset boundaries that are enforced. An abutting boundary communicates between a fluid and solid mesh; while, an overset boundary communicates between two overlapping fluid meshes.

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MS65

Verification of Partitioned Fluid-Structure Interaction Algorithms with Disparate Order of Accuracy

Specifying an appropriate and well-defined error metric to use along with a systematic grid study for a fluid-structure interaction code can be non-obvious. It can be especially difficult for a partitioned solver with disparate orders. This talk will focus on some of the common mistakes made by researchers when attempting to perform verification and it will present a well-defined error metric with a derived rate of convergence.

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MS65

A Stable Partitioned FSI Algorithm for Incompressible Flow and Deforming Beams

A new partitioned algorithm for coupling incompressible flows with elastic beams is described that overcomes the added-mass instability for light solids. The algorithm requires no sub-iterations and is fully second-order accurate. The new scheme is shown to be stable, even for very light beams, through the analysis of a model problem. The approach is then applied to the simulation of FSI problems involving beams undergoing large deformations using deforming composite grids.

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MS65

A New DG Interface Scheme for FSI

In this talk we examine a new method for coupling fluid and structural problems in a traveling wave problem that improves upon more standard algorithms.

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MS66

Estimating Network Degree Distributions from Sampled Networks: An Inverse Problem

Networks are widely used to model the relationships between elements in a system. Many networks observed today can be viewed as samples of a true underlying network. Hence, it is of fundamental interest to investigate the impact of the network sampling mechanism on the quality of characteristics estimated from the sampled network. We focus on the degree distribution as a fundamental network feature. Under a number of popular sampling designs, this problem can be stated as a linear inverse problem characterized by an ill-conditioned matrix. This matrix relates the expectation of the sampled degree distribution to the true underlying degree distribution and depends entirely on the sampling design. Approximate solutions can be provided through defining stable approximate inverses to the ill-conditioned matrix, the form of which we develop through the use of a classical penalized (generalized) least-squares framework. We present both theoretical and numerical results characterizing the performance of this approach, and illustrate the methodology in application to on-line social media networks.

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MS66

Synthesizing Social Networks From Random Walks

Networks are empirical snapshots of the past. We develop an application framework for generating interaction networks by means of different types of Random Walks. The characteristics of these networks are compared with the known theoretical and empirical graphs. We demonstrate that some random walks produce network topologies similar to small-world networks. The possibility of phase transitions in the graphs due to changes in the parameters of agent walks is the focus of this research.

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MS66

Improved Planted Clique Detection with Low-Rank Sparse PCA

Recent results have demonstrated a sharp threshold for planted clique detection with a simple algorithm based on principal component analysis (PCA) of a graphs modularity matrix. Sparse PCA of this matrix can successfully discover cliques where PCA-based detection methods fail. This presentation demonstrates detection of small planted cliques by applying sparse PCA to a low-rank approximation of the modularity matrix, illustrating the ability to detect smaller cliques when the semidefinite program is not computationally feasible.

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MS66

Identifying and Ranking Critical Interactions in Stochastic Dynamical Systems

The problem of designing efficient ways to control a noisy complex dynamical system is central to disciplines ranging

from the social sciences to physics. For example, which people should be immunised to ensure that an outbreak of infectious disease will not infect more than a fraction α of the population, or which elements of an infrastructure network should be prioritised for maintenance or protection? Because networks of interacting elements are a natural representation of complex systems, the problem can be cast in terms of identifying the most important interactions in an noisy interaction network. Here we introduce a mathematical framework that provides a unified representation for this class of problems; discuss mathematical and computational properties of the solutions; describe a scalable approximate solution technique with controllable precision; and compare its performance to recently published results on influence maximisation By placing the problem in this broader context, we connect it to decades of research in several disciplines, allowing us to apply general results about the computational complexity and error bounds of approximation methods.

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MS67

Using Performance Models to Manage Computation/Data Movement Tradeoffs in HPC Applications

With data movement costs becoming predominant over computation costs on modern machines, optimizations that involve more computation but less data movement are becoming popular. The range of possibilities is wide, so we need systematic ways to trade off computation and data movement to ensure benefits. In this talk, we discuss how we have made use of performance models as a means of managing tradeoffs between computation and data movement over a range of HPC applications.

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MS67

Data Centric Systems: Workflow Challenges and Opportunities

The volume, variety, velocity and veracity data is pushing how we think about computer systems. In this talk, I will describe the IBM Research Data Centric Systems work to develop systems that handle large data sets shortening time to solution. I will give an overview of our motivation, systems currently in design, and describe some of the challenges and opportunities these systems may have for workflows for application solutions setting the stage for this minisymposium.

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MS67

A Hierarchical Characterization of Scientific and Engineering Workflows Applied to Examples from the DoE and Other Communities

Workflows have always been used to describe jobs and applications progressing and interacting with systems. We have started an analysis by developing a workflow taxonomy with layers, describing the application stack, how we have used it for initial assessment of data use patterns, how they map to future needs, and the potential to develop lower layers to integrate with mapping of machine layers of workflows. As this evolves it brings in application and system performance collection, deriving workflow performance, and system monitoring as key initial capabilities. An overview of some workflows from the DoE Lab community using this methodology, studied at LANL and IBM Research will be presented.

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MS67

In-Memory Computing for Bioinformatics Pipelines

In life sciences applications such as DNA- and RNA-seq pipelines, the analysis is composed of a multistep analytical pipeline, which involves the output of one stage from the pipeline to be used as the input in the next stage of the pipeline, requiring multiple stages of reading in the input and writing the output to disk. Optimization of this pipeline by focusing on each separate module is thus not a very successful strategy; the bottleneck is in data movement, conversion of one data format to another and writing to the disk from one module followed by subsequent reading by the next stage of the pipeline. In this talk, we discuss the design and efficient implementation of a new data-centric framework to tackle data-intensive problems by storing the NGS and intermediate data in the interprocess memory regions of distributed nodes. The processes involved in the computation or analysis using this NGS data are subsequently relaunched on the same nodes and access the data in-memory, thus saving on costly disk I/O operations. We apply our new framework to parts of Trinity pipeline, demonstrating the improvement in performance in using such a framework for data-centric computing.

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MS68

Distributed PCA and Robust PCA

We study Principal Component Analysis (PCA) and Robust Subspace Recovery (RSR) in distributed settings. We consider a huge dataset in an ad hoc wireless sensor network, where each node has access only to one chunk of the dataset. The goal is to compute the PCA/RSR solution for the whole dataset, without transferring the data itself between the nodes. The presented work discusses Consensus Based Gradient/Subgradient and Consensus ADMM methods for both PCA and RSR. We provide efficient algorithms with fast convergence rates and theoretical justifications for Distributed PCA/RSR problems. To claim the usefulness of the algorithms we show some simulations for both synthetic data and some real world datasets, where PCA/RSR is applied as a data preprocessing step.

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MS68

LOBPCG-like Iterations in Eigenvalue-like Problems

Since introduction [A. Knyazev, Toward the optimal preconditioned eigensolver: Locally optimal block preconditioned conjugate gradient method, SISC, 2001(23), 517-541, DOI:10.1137/S1064827500366124] and efficient parallel implementation [A. Knyazev et al., Block locally optimal preconditioned eigenvalue xolvers (BLOPEX) in HYPRE and PETSc, SISC, 2007(29), 2224-2239, DOI:10.1137/060661624], LOBPCG has been used is a wide range of applications in mechanics, material sciences, and data sciences. We review some applications and extensions of the local optimality idea beyond standard eigenvalue problems.

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MS68

A Robust and Efficient Implementation of Lobpcg

Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) is widely used to compute eigenvalues of large sparse symmetric matrices. The algorithm can suffer from numerical instability if it is not implemented with care. This is especially problematic when the number of eigenpairs to be computed is relatively large. We present a number of techniques to improve the robustness and efficiency of this algorithm. We show that our approach consistently and significantly outperforms previous competing approaches in both stability and speed. We also present a robust convergence criterion which is backward stable.

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MS68

Preconditioned Solvers for Interior Eigenvalues of a Nonlinear Hermitian Eigenproblem

We consider preconditioned solvers for computing interior eigenvalues of a large-scale nonlinear algebraic Hermitian eigenproblem of the form $T(\lambda)v = 0$. The framework of the main algorithm, called preconditioned locally minimal residual (PLMR) method, arises from an extension of LOBPCG and enables several enhancements such as search subspace of larger dimensions, stabilized preconditioning, and refined Rayleigh-Ritz projections. With a good preconditioner, this algorithm is memory-efficient and exhibits rapid and robust convergence towards interior eigenvalues. PLMR can be also used to compute a large number of interior eigenvalues in a moving-window fashion, dramatically outperforming PCG methods.

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MS69

Window Selection in Dynamic Networks

Dynamic networks are a useful representation for a variety of learning tasks. Typically, these networks are constructed over an ad-hoc choice of window size. We show that not only can this choice significantly affect the performance of a given task, but that the notion of the 'right window size is task-dependent. We investigate how to find the best window size for a given task so that no ad-hoc choices need

be made.

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MS69

Using Local Methods to Robustify Graph-Based Learning

Local methods for graphs produce an output that does not depend on the entire graph. These are used in predicting the communities of a graph and inferring attributes through "guilt-by-association" methods and diffusion methods. I'll discuss how local methods help to make these tasks robust to errors that arose in the construction of network data based on non-network sources as well as errors in the supervised information used for attribute inference.

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MS69

Learning Opinion Dynamics in Social Networks

Social media and social networking sites have become a global pinboard for exposition and discussion of news, topics, and ideas, where social media users increasingly form their opinion about a particular topic by learning information about it from her peers. In this context, whenever a user posts a message about a topic, we observe a noisy estimate of her current opinion about it but the influence the user may have on other users' opinions is hidden. In this paper, we introduce SLANT, a probabilistic modeling framework of opinion dynamics, which allows the underlying opinion of a user to be modulated by those expressed by her neighbors over time. We then identify a set of conditions under which users' opinions converge to a steady state, find a linear relation between the initial and steady state opinions, and develop an efficient estimation method to fit the model parameters from historical fine-grained opinion and information diffusion event data. Experiments on data gathered from Twitter, Reddit and Amazon show that our model provides a good fit to the data and more accurate predictions than alternatives.

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MS69

Tissue-Specific Regulatory Circuits Reveal Variable Modular Perturbations Across Complex Diseases

We developed a comprehensive resource of 394 cell type- and tissue-specific gene regulatory networks for human, each specifying the genome-wide connectivity between transcription factors, enhancers, promoters, and genes. Integration with 37 genome-wide association studies (GWAS) shows that disease-associated genetic variants often perturb regulatory modules that are highly specific to disease-relevant cell types or tissues. Our resource opens the door to systematic analysis of regulatory programs across hundreds of human cell types and tissues: http://regulatorycircuits.org

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MS70

Data-Driven Model Reduction of Convection-Dominated, Unsteady Flows

It is well know that standard reduction techniques such as Proper Orthogonal Decomposition (POD) perform poorly for flows dominated by sharp gradients and shocks. In this work a novel Lagrangian orthogonal vortex blob decomposition is proposed for the reduction of convection-dominated, high-Reynolds number fluid flows. Similar to the POD approach, the proposed decomposition optimally reproduces the kinetic energy of the flow but unlike POD, the approach is demonstrated to accurately resolve sharp gradients and discontinuities.

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MS70

Krylov-Subspace Recycling via the POD-Augmented Conjugate Gradient Method

This talk presents a new Krylov-subspace-recycling method for efficiently solving sequences of linear systems of equations characterized by varying right-hand sides and symmetric-positive-definite matrices. As opposed to typical truncation strategies used in recycling such as deflation, we propose a truncation method based on a technique from nonlinear model reduction: goal-oriented proper orthogonal decomposition (POD). This idea is inspired by the observation that model reduction aims to compute a low-dimensional subspace that contains an *accurate* solution; as such, we expect the proposed method to generate a low-dimensional subspace that is well suited for computing solutions that can satisfy *inexact* tolerances. In particular, we propose specific goal-oriented POD 'ingredients' that align the optimality properties of POD with the objective of Krylov-subspace recycling. To efficiently compute solutions in the resulting 'POD-augmented' Krylov subspace, we propose a novel hybrid direct/iterative three-stage method that leverages 1) the optimal ordering of POD basis vectors, and 2) well-conditioned reduced matrices. Numerical experiments performed on solid-mechanics problems highlight the benefits of the proposed method over existing approaches for Krylov-subspace recycling.

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MS70

Krylov Subspace Recycling for Computing and Updating Reduced Order Models

Parameterized reduced order models provide a way to drastically reduce the cost of large inversion and optimization problems. However, in the course of the inversion/optimization, we may need to update the reduced order model as new data becomes available or if the model is no longer sufficiently accurate. Unfortunately, this may require the solution of many additional linear systems. To make this efficient, we consider new techniques, including using the reduced order model, to find good spaces for Krylov subspace recycling.

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MS70

A Mode Decomposition for Transport-Dominated and Parameter-Dependent Phenomena: The Shifted Proper Orthogonal Decomposition

Transport-dominated phenomena arise in various applications and provide a major challenge for common model reduction methods. We present the shifted proper orthogonal decomposition (sPOD) as an extension of POD by supplementing the modes with co-moving frames. This is accompanied by methods for detecting and separating different transport phenomena. We consider a reactive flow example with non-periodic boundary conditions and a parameter-dependent solution. We discuss the treatment of these two issues within the sPOD framework.

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MS71

Geometric Interpretations of Reduced Order Models

In his seminal work (1952) Mark Krein showed that the Stieltjes rational transfer functions can be equivalently presented by (Stieltjes) strings of point masses and weightless springs. In turn, the Stieltjes strings gave rise to interpretation of the ROMs via the second-order finite-difference approximation of the underlying PDE on judiciously chosen grids. I review applications of this approach and its generalizations to both forward and inverse problems and also outline some unresolved issues.

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MS71

Discrete Conductivity and Schroedinger Inverse Problems

We consider the problem of finding the electric properties of components in an electric circuit from measurements made at a few nodes. Such circuits can be used as reduced models of continuum problems. We give a condition based on the linearization of the problem that is sufficient to guarantee that the problem has a unique solution, except for a zero measure set. Our approach borrows ideas from the Complex Geometric Optics method that has been used to show uniqueness for continuum inverse problems.

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MS71

Computing Reduced Order Models for Diffuse Optical Tomography

To combat the computational bottleneck in diffuse optical tomographic imaging, we use a reduced order model (ROM) in the optimization to recover the parameterized absorption image. Constructing the ROM requires the solution of several full order problems to generate a candidate global basis. We introduce an inner-outer Krylov approach in which only incrementally new, relevant information is added to the existing global basis, and show the efficiency of our approach on examples.

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MS72

A Parallel Implicit Scheme for Geometric Nonlinear Elastic Equation Based on Weak Galerkin Finite Element Method

The aircraft design requires efficient massive parallel computing algorithm to solve fluid-structure interaction problem, particularly for the aeroelasticity. The implicit time marching scheme and domain decomposition are necessary for solving the geometric nonlinear elasticity equation. The novel developed weak Galerkin finite element method introduces a significant advantage to obtain optimal results and efficiency. We discuss about the theoretical background of weak Galerkin method, the design of parallel computing scheme and present the results.

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MS72

Weak Galerkin FEMs for Sensitivity Analysis for Elliptic Problems on Polyhedral Meshes

In this talk, we present preliminary results of sensitivity analysis on WG finite element methods for the Darcy equation on nonstructural meshes. For given quantities of interest, adjoint problems are solved and analyzed. Applications to the dependence of interstitial fluid pressure on vascular heterogeneity shall also be discussed. This is a joint work with Victor Ginting (UWYO) and Simon Tavener (ColoState).

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MS72

Basics of Weak Galerkin Finite Element Methods: Theory and Implementation

In the talk, the speaker shall discuss the basics of weak Galerkin finite element methods (WG) for partial differential equations, particularly on its theory and implementation. Weak Galerkin is a finite element method for PDEs where the differential operators (e.g., gradient, divergence, curl, Laplacian etc.) in the weak forms are approximated by discrete generalized distributions. The WG discretization procedure often involves the solution of inexpensive problems defined locally on each element. The solution from the local problems can be regarded as a reconstruction of the corresponding differential operators. The fundamental difference between the weak Galerkin finite element method and other existing methods is the use of weak functions and weak derivatives (i.e., locally reconstructed differential operators) in the design of numerical schemes based on existing weak forms for the underlying PDEs. Weak Galerkin is a natural extension of the classical Galerkin finite element method with advantages in many aspects. Due to its great structural flexibility, the weak Galerkin finite element method is well suited to most partial differential equations by providing the needed stability and accuracy in approximation.

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MS72

New Class of Finite Element Methods: Weak Galerkin Methods

Weak Galerkin (WG) methods are newly developed finite element methods. The methods use discontinuous piecewise polynomials on finite element partitions with arbitrary shape of polygons and polyhedrons. The purpose of this presentation is to introduce the basis concept of the WG methods and other important issues including implementations and applications of the the methods.

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MS73

Cancer Diagnostics and Prognostics from Comparative Spectral Decompositions of Patient-Matched Genomic Profiles

I will, first, briefly review our matrix and tensor modeling of large-scale molecular biological data, which, as we demonstrated, can be used to correctly predict previously unknown physical, cellular, and evolutionary mechanisms that govern the activity of DNA and RNA. Second, I will describe our recent generalized singular value decomposition (GSVD) and tensor GSVD comparisons of the genomes of tumor and normal cells from the same sets of glioblastoma brain and, separately, ovarian cancer patients. These comparisons uncovered patterns of DNA copy-number alterations that are correlated with a patient's survival and response to chemotherapy. Third, I will present our higher-order GSVD, the only mathematical framework that can create a single coherent model from multiple two-dimensional datasets, by extending the GSVD from two to more than two matrices.

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MS73

Exploiting Structure in the Simulation of Super Carbon Nanotubes

Super Carbon Nanotubes (SCNTs) can be modelled by a graph algebra, which encodes the structural and value symmetries present in these highly regular structures. We have developed an extremely space-saving, yet parallelizable, data structure called Compressed Symmetric Graphs (CSGs) which allows us to drastically reduce the amount of data that is needed to represent a SCNT by exploiting rotational and translational symmetry as well as order hierarchy and only storing non-symmetric parts while symmetric parts are dynamically reconstructed. This allows for a computationally efficient and space-saving computation of the stiffness matrix operator associated with SCNTs, even of higher order.

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MS73

Parallel Tucker-Based Compression for Regular Grid Data

As computing continues to trend towards the exascale, efficient use of computational resources is more important than ever. The scientific data produced by high fidelity simulations in combustion science and elsewhere are far too massive to store because even modest simulations produce terabytes of data. For typical scientific data, we have three spatial dimensions, a time dimension, and one other dimension corresponding to variables being tracked at each grid point. For instance, a modest simulation on a 3D grid with 500 grid points per dimension, tracking 100 variables, for 100 timesteps yields 5TB of data (assuming 4 bytes per value in single precision). We can view the data as a 5-way tensor and apply the Tucker tensor decomposition to find inherent low-dimensional structure. By taking advantage of the multiway structure, we are able to compress large-scale scientific data by a factor of 1000 or more with negligible loss in accuracy. However, working with such massive data requires a parallel implementation of the Tucker tensor decomposition. We explain the data distribution and algorithm and accompanying analysis. We apply the algorithm to real-world data sets to demonstrate the speed, compression performance, and accuracy of the method.

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MS73

A Revisit to the GEMM-Based Level 3 BLAS and Its Impact on High Performance Matrix Computations

The GEMM-based level-3 BLAS, by Kågström, Ling and Van Loan, is an effective way of handling the complex memory hierarchies present in HPC systems. By relying on a highly optimized general matrix multiply (GEMM) and suitable matrix partitionings, all the other level 3 BLAS can be defined in terms of GEMM and a small amount of level-1 and level-2 computations. After a quick review we will discuss the impact of the GEMM-based approach on new developments, e.g., recursive blocking, ATLAS BLAS and vendor libraries.

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MS74

High Frequency Boundary Integral Equations in a Linearly Stratified Medium

We present a high-order Nyström method for scattering from a smooth obstacle embedded in an unbounded continuously-graded medium, in which the square of the wavenumber varies linearly in the vertical coordinate. This models quantum particles in a uniform gravitational field, with broader applications in acoustics, optics and seismology. We approximate the Green's function exponentially accurately with wavenumber-independent effort via numerical steepest descent (quadrature) applied to a contour integral. 50λ diameter, 11 digits, in 1 minute.

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MS74

Multiple Traces Formulations: Novel Extensions and Challenges

Multiple Traces Formulations (MTFs) were developed in recent years to tackle wave scattering by heterogenous obstacles via boundary integral methods. For first kind MTFs, Galerkin discretization yields ill-conditioned matrices which require preconditioning to achieve convergence of iterative schemes with Calderón-type techniques being proved optimal. Still, the underlying use of dual meshes becomes prohibitively expensive very quickly. In this work, we introduce preconditioning alternatives based on more algebraic approaches while considering the properties of the boundary integral operators. We discuss their numerical efficiency and further improvements.

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MS74

Well-Posed Boundary Integral Equation Formulations and Nystrm Discretizations for the Solution of Helmholtz Transmission Problems in Lipschitz Domains

We present a general methodology that delivers well conditioned integral equation formulations for transmission problems in acoustics, electromagnetics, and elasticity. Our approach is based on certain approximations of Dirichlet to Neumann maps. We show that the new integral formulations are well posed in Lipshcitz domains and give ample numerical evidence that solvers based on these formulations are more competitive than solvers based on classical integral formulations of transmission problems.

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MS75

The 2d Euler Equations at Low Regularity

We will discuss a few recent results on propagation of low-degree regularity for the incompressible 2d Euler equations.

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MS75

The Vanishing Viscosity Limit in Porous Media

We consider the flow of a viscous, incompressible, Newtonian fluid in a perforated domain in the plane. We study the simultaneous limit of vanishing particle size and distance, and vanishing viscosity. Under suitable conditions on the particle size, interparticle distance, and viscosity, we prove that solutions of the Navier-Stokes system in the perforated domain converges to solution of the Euler system in the full plane. That is, the flow is not disturbed by the porous medium and becomes inviscid in the limit.

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MS75

Critical Regularity for Energy Conservation in 2D Inviscid Fluid Dynamics

We consider the issue of energy conservation for the 2D Euler system with an L^p-control on vorticity. A direct argument, based on a mollification in physical space, shows that the energy of a weak solution is conserved if $\omega = \nabla \times u \in L^{\frac{3}{2}}$. An example of a 2D field in the class $\omega \in L^{\frac{3}{2}-\varepsilon}$ for any $\varepsilon > 0$, and $u \in B^{1/3}_{3,\infty}$ (Onsager critical space) is constructed with non-vanishing energy flux, thereby establishing sharpness of the kinematic argument. Next, we prove that any solution to the Euler equations produced via a vanishing viscosity limit from the Navier-Stokes equations, with $\omega \in L^p$, for $p > 1$, conserves energy. We call such solutions *physically realizable* and we conclude that there is a mechanism preventing anomalous dissipation in 2D in Onsager supercritical spaces.

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MS75

On the Spectrum of Rayleigh-Taylor Instability in Presence of a Background Shear

We study instability and dynamics of an inhomogeneous stratified fluid in present of a background shear flow (Rayleigh-Taylor). This is a classical subject with a rich history. We show that the background shear stabilizes the essential spectrum of the linearized equation while retains discrete part. This observation allows to get rid of unfavorable short-wave instabilities and make possible to address the problem of non-linear instability by existing techniques.

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MS76

A Generalized Abs-Normal Form

A minor modification of the standard propagation rules from algorithmic differentiation allows the computation of a piecewise linearization for Lipschitz continuous functions that are given by a straight-line code, which only consists of smooth elemental functions and the absolute value. The piecewise linearization can be represented in terms of an abs-normal form. In this talk, we will examine this compact representation and point out some of its (dis-)advantages. Therefore, we will provide some simple examples that motivate an extension of the abs-normal form, which is also presented and discussed.

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MS76

Optimality or Convexity Conditions for Nonsmooth Objectives

The classical optimality conditions for smooth objective functions combine a stationarity condition with a local convexity condition. In the piecewise smooth case local convexity becomes subgradient regularity, which is far from being necessary for local optimality. We give necessary and sufficient conditions for either property. They are formulated in terms of matrices and vectors that can be evaluated by a slight extension of algorithmic differentiation to codes involving the absolute value primitive.

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MS76

Lexicographic Derivatives of Nonsmooth Systems

Nesterovs lexicographic derivatives provide useful first-order sensitivity information to methods for nonsmooth equation-solving and optimization. Unlike other established generalized derivatives such as Clarkes generalized Jacobian, lexicographic derivatives also obey sharp calculus rules. This talk describes efficient methods to compute lexicographic derivatives using variants of automatic differ-

entiation techniques. New relationships are also presented between the lexicographic derivative and the directed subdifferential of Baier, Farkhi, and Roshchina, thereby unifying these two approaches to generalized differentiation.

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MS76

Sensitivity Analysis of Nonsmooth Differential-Algebraic Equations

Nonsmooth differential-algebraic equations (DAEs) provide a natural framework for dynamic models of chemical processes exhibiting, for example, thermodynamic phase changes. Sensitivity analysis provides information which is useful in nonsmooth equation-solving (e.g., semismooth Newton methods) and dynamic optimization (e.g., bundle methods). However, these algorithms require an element of some class of generalized derivative, for which theoretical and computational approaches are currently lacking. In this talk, we detail new results regarding computationally relevant generalized derivatives of DAEs.

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MS77

Evaluating and Improving Sleep Spindle Detection Methods by SPEA2

Sleep spindles are intermittent, transient patterns of oscillation waves (11-16Hz) of brain activity during sleep as seen in human electroencephalographic (EEG) data. They are main features in classifying N2 stage of sleep and potentially useful biomarkers for various development, learning, and neurological disorders. Several automated spindle detection methods have been developed to improve the effectiveness and consistency of sleep spindle identification. We use evolutionary algorithms to optimize existing frequency-based sleep spindle detection algorithms.

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MS77

Game-Theoretic Transition Threshold in Hyperbolic Random Geometric Graphs

Hyperbolic random geometric graphs display power law distribution, short path lengths and high clustering coefficient, leading Boguna and others to propose that a hyperbolic geometry underlies the Internet graph. We use a game theoretic approach, based on the Prisoners Dilemma, to model diffusion in the network, examining network properties at the threshold between the persistence of cooperation and the complete adoption of defection.

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MS77

Variance-Reduced HMM for Stochastic Slow-Fast Systems

We propose a novel variance reduction strategy based on control variables for simulating the averaged equation of a stochastic slow-fast system. The right hand side of this averaged equation contains an integral with respect to the unknown invariant measure of the fast dynamics, which is approximated by the heterogeneous multiscale method (HMM). To improve the accuracy of HMM, which essentially is a MCMC method, we introduce a variance-reduced HMM estimator based on control variables.

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MS77

Constitutive Restrictions in Nonlinear Elasticity

The formal call for program of finding suitable restrictions on the form of response functions in nonlinear elastic materials so as to give physically reasonable behaviour in all possible deformations, the Hauptproblem, was proposed by Truesdell in 1955. Since then a lot of progress, yet far from complete, has happened. We will quickly review this classical problem. In order to quantify the notion stress increases with strain in an elastic material, which is one of possible restrictions, there are several constitutive inequalities that have been proposed in the literature. Due to some inherent shortcomings in them, which we will discuss, we proposed a new tensorial, frame-indifferent criterion for isotropic materials.

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MS77

Modeling Stripe Formation in Zebrafish: An Agent-Based Approach

Zebrafish have distinctive black and yellow stripes that form due to the interaction of different pigment cells. We present a two-population agent-based model for the development and regeneration of these stripes informed by recent experimental results. Our model describes stripe pattern formation, laser ablation and mutations. We find that fish growth shortens the necessary scale for long-range interactions and that iridophores, a third type of pigment cell, help align stripes.

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MS77
Infinite Dimensional Numerical Linear Algebra

Many numerical linear algebra problems come from a discretized, infinite dimensional linear system that has been truncated to "fit" on a computer. Is it possible to do numerical linear algebra on infinite dimensional matrices without truncating? It turns out that as long as the matrix is well structured, we can store it completely in a tailor-made data structure and perform some common algorithms. I will demonstrate a practical shifted QL algorithm for structured infinite matrices.

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MS78
Participants To Be Announced

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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MS79
An Optimization Approach to the Airlift Planning Problem

The United States Transportation Command (USTRANSCOM) is responsible for meeting the transportation requirements of the Department of Defense. Between sustainment for soldiers, humanitarian relief, and other worldwide missions, USTRANSCOM must regularly solve complex scheduling problems. Disruptions due to weather, maintenance, or unanticipated demand further complicate the process. To improve airlift planning, a new robust integer optimization-based approach has been developed. We describe the algorithm and demonstrate its performance and robustness for an example application problem. This work was sponsored by USTRANSCOM under Air Force Contract No. FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.

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MS79
Target Identification in Sonar Imagery Via Simulations of Helmholtz Equations

We present a multiscale approach for identifying objects submerged in ocean beds by solving inverse problems in high frequency seafloor acoustics. The setting is based on Sound Navigation And Ranging (SONAR) imaging used in military, engineering, and scientific applications. The forward model incorporates simulations, by solving Helmholtz equations, on a wide range of spatial scales, allowing for detailed recovery of seafloor parameters including the material type. In order to lower the computational cost of large-scale simulations, we take advantage of a library of representative acoustic responses from various seafloor parametrizations.

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MS79
Modeling Tides in the West Pacific

This talk explores the challenges encountered in creating a tidal model for the South China Sea and greater Pacific region. We discuss the determination of optimal friction values using uncertainty quantification techniques. Model evaluation is performed by comparing amplitudes and phases of major tidal constituents at stations from various sources. This work is a joint academic/industry project with the University of Notre Dame and FM Global.

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MS79
Analysis of Hyperspectral Images Via Difusion Methods on Graphs

First, we present a novel method for automated anomaly detection in auto-fluorescent retinal images provided by the National Institute of Health (NIH). This work is motivated by the need for new tools to improve the capability of diagnosing macular degeneration in its early stages, track the progression over time, and test the effectiveness of new treatment methods. The method we propose is a combination of a nonlinear dimensionality reduction on graphs, along with a new classification method. Comparison to other schemes shows that this novel method yields the highest rate of accurate anomaly detection. We also show that the dimension reduction algorithm that I used is in the family of kernel-based techniques, a set of Harmonic Analysis tools for graphs. Finally and as an example, we introduce a new system in this family.

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MS80

A Numerical Homogenization Method for Composite Dispersive Materials

We present a numerical homogenization method to compute effective parameters, such as permittivities and relaxation times, for composite dispersive materials in which the wavelength of the electromagnetic field is much larger than the relevant dimensions of the microstructure. The numerical method is based on the periodic unfolding method for simulating the electromagnetic field in a composite material exhibiting heterogeneous microstructures described by spatially periodic parameters. Examples are presented using the Debye and Lorentz dispersive media models.

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MS80

Anisotropic Material Based FDTD Method for Dispersive and Complex Media

A novel Maxwell solver was developed based on the use of anisotropic material and coordinate mapping. A key feature is the invariance of Maxwell equations under coordinate transformation. Subgridding can be achieved by mapping non-orthogonal grid to logically rectangular mesh and then numerically solved using a stable anisotropic FDTD algorithm. In this talk, we will discuss the recent progress of the anisotropic material based FDTD method and its extension to dispersive and complex media.

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MS80

Charge-Conserving Electromagnetic Particle-in-Cell Algorithms on Unstructured Grids Based on Differential Forms

We present an electromagnetic particle-in-cell algorithm with exact charge-conservation properties on unstructured (irregular) grids. Charge conservation is derived from first principles by using the exterior calculus of differential forms to represent field, currents, and charges as differential of various degrees. The use of exterior calculus provides precise localization rules for the dynamic variables on the various grid elements (nodes, edges, facets). Charge conservation is obtained without the need for any post-processing steps. Whitney forms are used as interpolants from discrete differential forms to continuum space, and to derive Hodge star operators (i.e., mass matrices incorporating all metric information about the finite element grid). The field update is based on the first-order coupled Maxwells curl equations to avoid spurious modes with secular growth. We provide numerical examples involving travelling-wave tube amplifiers designed to harness bunching effects from Cherenkov radiation.

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MS80

Time Domain Interface Methods for Electromagnetic Wave Propagation in Dispersive Media

Across the dispersive interfaces, the electromagnetic fields loss the regularity in a frequency-dependent or time-varying manner, which impose a great difficulty in FDTD simulations. In order to track these transient jumps, we have developed novel Maxwell systems for both Debye and Drude media in TM and TE modes. The resulting time-dependent jump conditions are enforced via the matched interface and boundary (MIB) scheme. High order convergences are numerically confirmed.

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MS81

The Shifted Nitsche Method: A New Approach to Embedded Boundary Conditions

Embedded boundary methods obviate the need for continual re-meshing in many applications involving rapid prototyping and design. Unfortunately, many finite element embedded boundary methods for incompressible flow are also difficult to implement due to the need to perform complex cell cutting operations at boundaries. We present a new, stable, and simple embedded boundary method, which we call the shifted Nitsche method, which eliminates the need to perform cell cutting, and demonstrate it on large-scale incompressible flow problems.

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MS81

The Shifted Immersed Boundary FEM Method for FSI

The immersed boundary method drastically simplifies grid generation, and, for this reason, is a powerful tool for fluid-structure interaction computations. However, integration over cut elements suffers from the well-known small cut-cell issue. We propose a new immersed boundary finite element method, in which boundary conditions are imposed through the shifted Nitsche method on two surrogate discrete boundaries, lying on the interior and exterior of the true boundary interface. We then construct appropriate force-averaging operators, with the purpose of preserving smoothness in the computed solutions.

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MS81

An Added Mass Partitioned FSI Algorithm for Rigid Bodies and Incompressible Flows

A stable added-mass partitioned (AMP) algorithm is developed for fluid-structure interaction (FSI) problems involving viscous incompressible flow and rigid bodies. The algorithm remains stable, without sub-iterations, even for light rigid-bodies when added-mass and viscous added-damping effects are large. A second-order accurate implementation of this AMP scheme is developed based on a fractional-step method for the incompressible Navier-Stokes equations using finite difference methods and overlapping grids to handle the moving geometry. The numerical scheme will be verified on a number of benchmark problems.

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MS81

FSI in Multi-Phase Flows Using An ALE/Phase-Field Formulation

We present a phase-field/ALE method for simulating fluid-structure interactions (FSI) in multi-phase flow. We solve the Navier-Stokes equation coupled with the Cahn-Hilliard equation and the structure equation in an arbitrary Lagrangian Eulerian (ALE) framework. For the fluid solver, a spectral/hp element method is employed for spatial discretization and backward differentiation for time discretization. For the structure solver, a Galerkin method is used in Lagrangian coordinates for spatial discretization and the Newmark-β scheme for time discretization.

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MS82

Iterative Sample Removal for Reliable Networks

Inferring domain-specific signals from large-scale raw data is one of the most challenging problems in analyzing biological data. In the absence of methods to identify simple causative signal, correlation network analysis represents a viable alternative approach for inferring regulatory relationships. However, the lack of recognized validation in many of such studies has limited the impact of the results obtained from correlation networks. In this research, we propose a methodology to measure the quality of the results obtained from the analysis of correlation networks. We investigate how individual samples affect the robustness of the network model, and develop a schema to test the impact of individual sample removal as the computational load grows.

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MS82

Noise in Networks: Future Directions

The organizers will lead a discussion, with participation from the other speakers and attendees, on the current state of research on analysis of networks with noise and uncertainty, and possible future directions. The discussion will focus on the implications of network noise from a theoretical perspective, and its impact in different applications, including the ones presented. A key point will be the interplay between algorithms and statistics in this emerging subfield of network science.

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MS82

Evolution of Co-authorship Networks as Measure of Interdisciplinarity

Obscured and false nodes in networks coupled with variability in edge type pose wide range of challenges in network analysis. Here, we present a case study based on co-authorship networks of Arizona State University before and after its New American University transformation. At the core of the transformation is focus on interdisciplinary research. We characterize various types of noise in the co-authorship networks along with their impact on network properties. We, then, leverage temporally evolving network properties to quantify emergence of interdisciplinarity. This talk highlights macroscopic network structure that leads the way toward identifying and understanding the crosstalk between disciplines using Web of Science records.

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MS82

Stability and Continuity of Centrality Measures in Weighted Graphs

We introduce formal definitions of continuity and stability for node centrality measures in weighted graphs. We show that the frequently used measures of degree, closeness and eigenvector centrality are stable and continuous whereas betweenness centrality is neither. Through numerical experiments in synthetic and real-world networks, we demonstrate that both stability and continuity are desirable in

practice since they imply different levels of robustness in the presence of noisy data. In particular, a stable alternative of betweenness centrality is shown to exhibit resilience against noise while preserving its notion of centrality.

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MS83

Successive Convolution: a High Order Framework for Pdes Based on the Method of Lines Transpose

Abstract Not Available at Time of Publication

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MS83

A Numerical Framework for Integrating Deferred Correction Methods to Solve High Order Collocation Formulations of ODEs

In this talk, we study the deferred correction methods by separating two different concepts: (1) the properties of the **converged solution** to the collocation formulation, and (2) the **convergence procedure** utilizing the deferred correction schemes to iteratively and efficiently reduce the error in the provisional solution. This new viewpoint allows the construction of a numerical framework to integrate existing techniques, by (1) selecting an appropriate collocation discretization based on the physical properties of the solution to balance the time step size and accuracy of the initial approximate solution; and by (2) applying different deferred correction strategies for reducing different components in the error of the provisional solution. We discuss properties of different components in the numerical framework, and presents preliminary results on the effective integration of these components for ODE initial value problems.

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MS83

An Integral Equation Approach to Solving the Navier-Stokes Equations Via Rothe's Method

We present a Rothe's Method, integral equation approach to solving the two dimensional incompressible Navier-Stokes equations in a pure stream-function formulation. There are multiple advantages of such an approach, not the least of which are: the velocity is automatically divergence free, and complicated (nonlocal) boundary conditions for the vorticity are avoided. Applying a semi-implicit, temporal discretization scheme yields a sequence of boundary value problems for the modified biharmonic equation. A system of Fredholm second kind integral equations is constructed for the modified biharmonic equation with gradient boundary conditions. This formulation is highly amenable to acceleration via fast algorithms such as the fast multipole method or fast direct solvers, resulting in optimal computational complexity. Further development of this approach will be discussed.

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MS83

Method of Lines Transpose Applied to Regularized Kernels

We consider the motion of a collection of particles, where the force is given by Coulomb's law. If using a high-order time integrator, the accuracy quickly deteriorates if two particles come close to one another. By regularizing the potential function, high-order accuracy to a nearby problem can be achieved. I will describe a new class of regularizations that allow for high-order accuracy and only slightly changing the original problem.

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MS84

Data Management on the GPU Using OpenMP 4

GPU computing usually offers impressive bandwidth and flops, but moving and allocating data between the CPU and GPU can be time consuming and difficult to program. Combine that with learning a new GPU specific language and the task of moving code to the GPU can be high. Fortunately, the OpenMP 4 programming model allows the use of target directives to easily offload data and computations onto a target device and the IBM compiler research team has been implementing OpenMP 4 target offloading for Nvidia GPUs. This OpenMP 4 functionality is freely available as a branch of the open source LLVM compiler. Importantly, OpenMP 4 allows the same code to run on the host (CPU) or the target (CPU) without needing to recompile. In this presentation I will explain the mapping syntax and show some results from applications where LLVM and

OpenMP 4 has been used to map data and computations onto the GPU.

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MS84

The Seismic Stress Test for Data Centric Systems

Vector data recording technology has advanced to the point that elastic wave equations are now the method of choice and the near future will require full field stress based methods. The directions of principal stress will be used to determine geological features, like fractures. Data will drive the solution processes - the order magnitude increase of field data - will need the capabilities of data centric computing. We will illustrate seismic algorithms that will best operate on data at the cpu/gpu level and at the data storage level.

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MS84

Moving Molecular Data for Mobile Visualization

Petabytes of molecular simulation data become a case study for data centric computing. Can the data be efficiently moved for remote visualization for globally distributed input for computational steering? Bandwidth into mobile devices becomes a system design issue. There are significant implications for geometric modeling and attendant numerical analyses. We present supportive work on modeling entries from the Protein Data Bank by Bézier curves, as driven by data volume and velocity.

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MS84

Data Centric Workflow of Industrial and Global Seismic Processing, Imaging and Inversion

To develop high-resolution images of subsurface resistors and the whole Earth's interior, the size of I/O and computation becomes considerably large in the workflow of industrial and global seismic data processing and imaging. The I/O performance creates the bottlenecks in the optimizing the workflow. In this talk, we discuss the possibility of optimizing the workflow by integrating parallel I/O libraries and new data formats in the workflow, stores data in main memory, and transparently spills over to other storage, like local flash memory or the parallel file system. The benefits is to reduce I/O and computation time of the workflow.

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MS85

Inferring Roles of People in Social Networks Extracted from New York Times Articles

We build networks from a collection of New York Times articles using named entity recognition and two different techniques, co-occurrence and neighborhood. Our goal is to measure the impact each technique has on predicting the role of people in the network. We present and contrast results on the role prediction task using network analytics, text-based features, and multiple classifiers. We show that a person's role can be predicted with good accuracy using these techniques.

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MS85

Mis-Specification, Sparsity, and Superpoplulation Inference for Sparse Social Networks

Recent interest in network data has driven a flurry of research into generative network models. These models have a mixed record in scientific application. In particular, there is a disconnect between two of the major use cases for network models. In this paper, we develop a theoretical framework for the network superpopulation inference problem and use it to understand why many network models are ineffective at predicting, comparing, or sharing information across network samples.

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MS85

Networks in Neuroscience and Climate Science

The complex network paradigm is increasingly being pursued in the analysis of spatio-temporal data that is collected in both neuroscience and climate science. Advances in these domains have processed independently, despite the similarity in the challenges faced due to the underlying spatio-temporal nature of the data. In this talk, I will present common data science problems that are studied in these two domains and the different directions that are being pursued.

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MS85

Do I Have the 'Right' Network? Task-Oriented Models for Network Structure Inference and Vali-

dation

Networks modeling real datasets often contain overlapping latent relationships. We first demonstrate that while we can learn a network representation optimized for a particular task, these networks perform poorly on other tasks. Therefore, finding the best representation across *all* tasks performs poorly on *many* of them. Rather than discovering this single "most robust' network representation, this work aims to discover *axes* on the space of potential networks by analyzing the biases of different network inference methods, modeling *difficult* subnetworks across different tasks.

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MS86

Analysis and Control of Pre-Extinction Dynamics in Population Networks

Extinction risk is an important question in both population and ecological community dynamics. We observe that in stochastic population models, the intrinsic noise can cause random switching between metastable states before the population goes extinct. Modeling the dynamics of the network of metastable states may provide insight to the complex behavior of the system. Using this framework, we can understand pre-extinction cycling dynamics and quantify the impact of control methods to decrease the mean time to extinction.

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MS86

Using the Wentzell-Freidlin Least Action to Maneuver Network Dynamical Systems

We present a scalable, quantitative method based on the Wentzell-Freidlin least action to predict and control noise-induced switching between different states in genetic networks that can also direct transitions between stable states in the absence of noise. We apply this method to models of cell differentiation and apoptosis, showing how it can identify potential targets that manipulate the system dynamics.

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MS86

Does Delay Constructively Influence the Dynamics of Genetic Networks?

Bistability is a central characteristic of biological switches. It is essential in the determination of cell fate in multicellular organisms, the regulation of cell cycle oscillations during mitosis, and the maintenance of epigenetic traits in microbes. Since gene expression is stochastic, bistable genetic networks can randomly switch between metastable states (noise-induced transitions). We study the impact of transcriptional delay and the cell cycle on the dynamics of bistable genetic networks. We find that transcriptional delay dramatically stabilizes such networks and that noise-induced transitions between bistable states concentrate near the beginning of the cell cycle (just after cell division). To explain these findings, we introduce and analyze a 5-states symbolic model with discrete- and continuous-time stochastic components.

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MS86

The Force of Fluctuations: from Analysis to Control in Extinction and Switching in Networks

Noise in various forms is known to cause switching between states, create new meta-stable states, and form global dynamical structures. In this talk, I will review some previous work on the effects of noise in static and adaptive networks, and show how to extend the theory to heterogeneous networks with a specified degree distribution. Applications will be to delay-coupled swarms and epidemic spread and control in large populations.

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MS87

A Model Reduction Approach to Inversion for a Parabolic Partial Differential Equation

I will describe a novel numerical inversion method for a parabolic partial differential equation arising in applications of control source electromagnetic exploration. The unknown is the electrical resistivity in the earth and the data are time resolved measurements of the magnetic field. The method described uses model reduction ideas and has been implemented in one and two dimensions.

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MS87

Nonlinear Seismic Imaging via Reduced Order Model Backprojection

We introduce a novel nonlinear seismic imaging method based on reduced order models (ROMs) that project the wave equation propagator on the subspace of wavefield snapshots. These ROMs can be computed entirely from the time domain seismic data. The image is a backprojection of the ROM using the subspace basis for a known kinematic velocity model. Nonlinear implicit orthogonalization of wavefield snapshots differentiates our approach from conventional linear methods. It removes automatically the multiple reflection artefacts and doubles the resolution in range direction compared to conventional reverse time migration.

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MS87

Equivalence of Spectrally Matched Grids and Galerkin Methods

It was known earlier that reduced order models (in the form of three point finite difference schemes) which are chosen to match data in the spectral domain are equivalent to spectral Galerkin methods at the boundary. We discuss now how to compute the Galerkin basis which yields the same reduced system everywhere in the domain. This implies that the entries of the reduced order model systems generated from data can be directly related to integrals of the coefficient, which has the potential yield new direct methods for inversion.

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MS87

A Model Based Data Driven Dictionary Learning for Seismic Data Representation

Abstract Not Available at Time of Publication

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MS88

Molecular and Physical Mechanisms of Fibrinolysis: Modeling and Experimentation

Fibrinolysis is the enzymatic degradation of blood clots. Due to the complexity of the fibrinolytic system, mathematical models can be used to identify fundamental mechanisms underlying fibrinolysis. Laboratory experiments coupled with our previously published stochastic multiscale model of fibrinolysis yield important insights relating to clot degradation rate, effective diffusion of molecules through the clot, and improved stroke treatments.

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MS88

Microorganisms Swimming Through a Compliant Viscoelastic Network

Microorganisms swim through viscous fluids with suspended polymeric networks whose length scales are comparable to the organism's. A model of a flagellar swimmer moving through a compliant viscoelastic network immersed in a 3D viscous fluid will be presented. The network links are stretched or compressed in response to the fluid flow caused by the organism, and these elastic deformations also affect the fluid motion. We find that stiffer networks give a boost to the velocity of the swimmer and that the swimming efficiency depends on the evolution of the compliant network as the swimmer progresses through it.

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MS88

A Mathematical Model of Venous Thrombosis Initiation

Unlike arterial thrombosis, venous thrombosis starts without vascular injury. It proceeds on a time scale much slower than arterial thrombosis. We present a model accounting for the cellular and protein interactions thought important in venous thrombosis, as well as the role of flow-mediated transport. We use it to explore the interplay between pro- and anti-thrombotic factors, how their imbalance can initiate venous thrombosis, and what accounts for the difference in time scales.

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MS88

Numerical Methods for Micro-Structure Evolution of Materials

In this talk, we will introduce the nonlinear PDEs that are commonly used to model micro-structure evolution of materials. We will go over the current available numerical methods to solve such PDEs. We will also present a new computational framework that is accurate, efficient and easy to adapt to a large class of problems with an energy minimization structure.

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MS89

Impact of Single-Neuron Dynamics on Transfer of Correlations from Common Input

One ubiquitous source of spike train correlations in the nervous system is common input. How input correlations map onto output spike correlations is complex, depending on single-neuron dynamics in subtle ways. I will describe significant trends that can be be quantitatively related to single-cell characteristics, demonstrate how these properties modulate the firing rate of downstream populations, and describe on-going work in which we generalize these findings to recurrent networks.

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MS89

Emergence of Limit Cycles In Simplified Basal Ganglia Model

The basal ganglia is a complicated interconnected system of nonlinear firing neurons. Simplifying this system with the use of piecewise-linear differential equations splits the space up into 27 different regions. These modified equations, are able to solve the system exactly in each individual region, while still keeping the original global nonlinear structure. By exploiting the the system's region boundaries we are able to show the existence of limit cycles cases in addition to stability cases.

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MS89

Synchrony Among Chemically and Electrically Coupled Neurons

Global oscillations, which are linked to synchronized neuronal activity, are known to exist in brain networks. Though little is known about the mechanism behind the generation of these oscillations, researchers believe that electric coupling through sites called gap junctions may facilitate their emergence. Following data from experiments, we construct a detailed model with synaptic and electric coupling using a modified version of the Hodgkin-Huxley equations. We use this model to analyze the resulting dynamical regimes.

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MS89

Firing-Rate Model of Locust Antennal Lobe

Using a coarse-graining approach, we formulate a mathematical model to describe the possible underlying mechanisms by which insects detect and identify odors. The resulting firing-rate model incorporates the slow and fast conductance timescales believed to play a vital role in the network behavior of the locust antennal lobe. The fast dynamics arise as an attracting limit cycle, followed by a pause in activity due to the slow variable, before a much slower oscillatory pattern reemerges.

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MS90

Optimal Design of a Bioremediation System for Water Resources

In Situ Chemical Oxidation (ISCO) for remediation of contaminated groundwater is a common method for cleaning up groundwater contaminated by chlorinated and recalcitrant compounds. For certain sites, oxidant encapsulated in paraffin wax cylinders is well indicated. The release of oxidant from the cylinders, groundwater flow, and contaminant-oxidant interaction is modeled based upon well-understood concepts of hydrogeology, field tests, as well as laboratory tests. Two different simulators approach the solving of the resulting system of PDEs in a different ways, one using finite difference approximation and the other using a Radial Basis Function coallocation method (RBFcm). Verification of the models and a sensitivity analysis of site parameters have been conducted with an eye towards creating a tool to optimize the placement of cylinders and cost of clean-up.

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MS90

Analysis of Farming Processes Using Simulation-Based Optimization

We describe a framework to aid policy makers, farmers, and other community members in their efforts to understand, quantify, and assess the often competing objectives water consumers have with respect to usage. The foundation for the framework is the construction of a simulation-based optimization software tool using two existing software packages. In particular, we couple a robust optimization software suite (DAKOTA) with the USGS MF-OWHM water management simulation tool to provide a flexible software environment that will enable the evaluation of one or multiple (possibly competing) user-defined (or stakeholder) objectives. We present numerical results for case studies related to crop portfolio management with several defined objectives. The objectives are not optimally satisfied for any single user class, demonstrating the capability of the software tool to aid in the evaluation of a variety of competing interests.

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MS90

Exploiting Infiltration Events: Management of Recharge Networks

Networked groundwater recharge basins have been used extensively for management of stormwater, particularly when new developments are constructed and the developer must respond to federal and state regulations requiring limited runoff after storm events. More recently, these networks are being considered for management of groundwater resources, both to mitigate the effects of salt-water intrusion into near-shore drinking water wells and to replenish aquifers that have sustained years (and often decades) of over draught. In this work, we investigate the use of optimization strategies to help ground water management agencies determine the appropriate size and location of a recharge basin network. We consider differing objective functions, from economic and environmental view points, and appropriate software tools for modeling and evaluating the performance of the network.

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MS90

Lyme Disease in New York - Modeling Multi-level Population Interactions as Affected by Human Driven Development

The prevalence of Lyme Disease continues to grow in North America, not only in geographic extent but also with respect to number of cases, disease burden and other economic impacts. Although the spatial spread of the disease focuses on the dynamics at low population levels, we seek to understand the potential implications of endemic levels. In particular, we want to understand what mechanism might be in play that control the tick population levels — the key driver with respect to morbidity rates.

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MS91

Finite Element Multigrid Framework for Mimetic Finite Difference Discretizations

We are interested in the efficient multigrid method of linear systems of equations discretized from the mimetic finite difference (MFD) schemes which work on general unstructured and irregular grids and result in discrete operators that satisfy the exact sequence connecting grad, div and curl operators on the continuous level. We derive such MFD schemes from the standard finite element spaces. Using the finite element framework, we are able to analyze the convergence of the MFD discretizations and construct efficient multigrid methods for the MFD discretizations of elliptic partial differential equations based on the Local Fourier analysis. Finally, we present several numerical tests to demonstrate the robustness and efficiency of the proposed multigrid methods.

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MS91

Meshing and Fem Simulation of Ion Transport in Protein Channels and Nanopores

Mesh generation for biomolecules and algorithm stability are still technical difficulties preventing application of continuum models to molecular simulation. Our recent developments will be reported, especially for modeling ion transport in channel proteins and nanopores. A webserver is designed to help users avoid most of the technical difficulties encountered in setting up and simulating complex systems.

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MS91

Providing User Interfaces for Mesh Generation and Simulations Using Computational Model Builder (CMB)

One of the major challenges associated with simulation workflows has been providing end-users with custom graphical user interfaces for accessing meshing and simulation technologies. The Computational Model Builder (CMB) project is an open source effort to quickly produce these interfaces for defining simulation input decks as well as driving meshing processes. This presentation will present the architecture of CMB as well as examples of interfacing with various meshers and simulations.

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MS91

A Posteriori Error Analysis and Efficient Discretization for Two-Stage Time Integration Methods and the Parareal Algorithm

A common approach to solving partial differential equations is to discretize in space producing a large system of ODEs. We consider numerical methods for initial value problems that employ a two stage approach. We develop an adjoint-based a posteriori error analysis which enables a novel approach for constructing Stage 2 discretizations that accounts for cancellation of error. We extend our analysis to derive estimates and discretization strategies for the (parallel-in-time) Parareal Algorithm.

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MS92

The Efficient Computation of Dense Derivative Matrices in MATLAB Using ADMAT and Why Sparse Linear Solvers Can Help

It is well accepted that sparse derivative matrices, Jacobians or Hessians, can be efficiently computed using automatic differentiation by cleverly exploiting the sparsity, often by taking a graph coloring point of view. Such methods appear not to be applicable to many compute-intensive problems such as control problems, design, and inverse problems because such application classes do not yield sparse Jacobian or Hessian matrices. Therefore, while AD can be applied it will be very expensive (similar to finite differencing) if directly applied to the objective function. We show that such common important problems exhibit structure and within that structure, hidden sparsity. AD can be tailored to take advantage of this, including the use of sparse linear solvers, to great efficiency gains. We illustrate this, and demonstrate the use of new easy-to-use templates for use with ADMAT in the MATLAB environment.

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MS92

Charlie Van Loan and the Matrix Exponential

The matrix exponential started to be treated as a serious computational tool in the late 1960s. Some of the most influential work on e^A is that by Charlie Van Loan. His 1978 paper *Nineteen Dubious Ways to Compute the Exponential of a Matrix*, with Cleve Moler, is well known, but Charlie made several other important contributions to the subject. I will describe Charlie's e^A contributions and explain how numerical methods for e^A have advanced to the current state of the art.

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MS92

Nineteen Dubious Ways to Compute the Zeros of a Polynomial

In the spirit of the 1978 and 2003 papers by Moler and VanLoan in SIAM Review, "Nineteen Dubious Ways to Compute the Exponential of a Matrix", I will examine a few well known, and a few not so well known, methods for computing the zeros of a univariate polynomial. One of the methods, which originated with the "roots" function in MATLAB, reverses the role played by the companion matrix in traditional Linear Algebra.

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MS92

On Rank-One Perturbations of a Rotation

The following problem arises in computer vision. Find a rotation matrix R and a matrix B of rank one such that a given matrix A, known to have this form (up to measurement errors), satisfies A = R + B. A related problem is to find R and B such that R + B is the closest rank-one perturbation of a rotation to the given matrix. The problem was solved using geometric arguments in a classic paper in the vision literature. I will give it an algebraic, SVD-based treatment, and correct a numerical accuracy problem present in the previous treatment. I'll also relate the pivotal role played by Charlie Van Loan in the publication of the paper.

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MS93

Recent Progress on Fast Algorithms for Oscillatory Problems from Density Function Theory

In this talk, we will discuss some recent progress on developing fast algorithms for oscillatory problems in density function theory calculations.

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MS93

Interconnected Hierarchical Structures for Solving Non-coercive Elliptic PDEs

We present a direct method for solving discretized elliptic PDEs. Based on a multilevel domain partitioning, we propose a way to form consistent hierarchically semiseparable matrices across different levels of subdomains. The representation reuses the basis from lower-level compression results. This improves the speed and the accuracy by avoiding existing recompression procedures. One major application is the Helmholtz equation with many wavelengths. This is joint work with Maarten V. de Hoop and Jianlin Xia.

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MS93

Fast Huygens Sweeping Methods for High Frequency Waves in Inhomogeneous Media

Starting from Babich's expansion, we develop a new high-order asymptotic method, which we dub the fast Huygens sweeping method, for solving point-source Helmholtz equations in inhomogeneous media in the high-frequency regime and in the presence of caustics. The first novelty of this method is that we develop a new Eulerian approach to compute the asymptotics, i.e. the traveltime function and amplitude coefficients that arise in Babich's expansion, yielding a locally valid solution, which is accurate close enough to the source. The second novelty is that we utilize the Huygens-Kirchhoff integral to integrate many locally valid wavefields to construct globally valid wavefields. This automatically treats caustics and yields uniformly accurate solutions both near the source and remote from it.

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MS93

Optimized Helmholtz Discretizations: New Applications and a Connection to Geometrical Optics

We construct geometrical optics solutions for finite-difference discretizations of the Helmholtz equation. We present a finite-difference discretization of the Helmholtz equation in which highly accurate geometrical optics phases and amplitudes are obtained on relatively coarse meshes. This makes it possible to use coarser meshes for certain Helmholtz problems. The method can also be used to improve the efficiency of multigrid-based solvers.

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MS94

Determining Wavenumber for Fluid Equations

Abstract Not Available at Time of Publication

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MS94

The Aggregation Equation with Newtonian Potential

The aggregation equation with Newtonian potential models several different physical problems, including chemotaxis (when diffusion is present) and type-II superconductivity (without diffusion). In this talk, we apply techniques from two-dimensional fluid mechanics to investigate well-posedness theory and the inviscid limit for a generalization of this equation.

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MS94

The Vanishing Alpha Limit of Incompressible Euler-Alpha

In this talk we examine recent results concerning the limit $\alpha \to 0$ of solutions to the Euler-α model in bounded two-dimensional domains. We consider both the Navier friction case and the no-slip case.

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MS94

The Van Dommelen and Shen Singularity in the Prandtl Equations

In 1980, van Dommelen and Shen provided a numerical simulation that predicts the spontaneous generation of a singularity in the Prandtl boundary layer equations from a smooth initial datum, for a nontrivial Euler background. In this paper we provide a proof of this numerical conjecture by rigorously establishing the finite time blowup of the boundary layer thickness.

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MS96

Improved Solvers for the Time Harmonic Maxwell Equations on Axially Symmetric Domains

This talk presents improved solver for time harmonic Maxwell Equations on axially symmetric domain. The new integral equation based solution technique is capable of handling various boundary singularities and boundary conditions. While the solver has nearly optimal complexity, the method is robust and is able to obtain high accuracy.

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MS96

Recent Developments in Fast and Robust Algorithms for Quadrature by Expansion (QBX)

Efficient implementations of Fast Multipole Methods (FMMs) are essential for developing linear CPU time layer potential evaluators. In the QBX environment, computing local expansions and increasing the order of expansions tends to slow the FMM down. We present a faster version of the FMM using precomputed skeleton bases to represent outgoing and incoming expansions, and optimized diagonal form translation operators for converting outgoing expansions to incoming expansions. The algorithm's effectiveness is demonstrated via several numerical examples.

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MS96

On the Solution of Elliptic Partial Differential Equations on Regions with Corners

In this talk we investigate the solution of elliptic partial differential equations on domains with corners. We observe that, in the vicinity of corners, the solutions to the boundary integral equations of classical potential theory are representable by linear combinations of certain non-integer powers of x, where x is the distance from the corner. In addition to being analytically perspicuous, the resulting expressions lend themselves to the construction of accurate and efficient numerical algorithms. We illustrate the results by a number of numerical examples.

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MS96

Harmonic Polynomials and Quadrature by Expansion

Quadrature by expansion (QBX) is a method for evaluation of boundary integral equations that is high order, kernel independent, and amenable to acceleration. The spectral behavior of QBX is important for computing solutions to boundary value problems both accurately and quickly. For the case of the double layer potential kernel, we describe an approach to analysis of the spectral behavior of QBX based on density functions that give rise to polynomial solutions.

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MS97

A Galerkin Radial Basis Function Method for Nonlocal Diffusion

Abstract Not Available at Time of Publication

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MS97

Numerical Study of Space-Time RBF for PDEs

We are experimenting with space-time radial basis function methods for the numerical solutions of time-dependent PDEs. Unlike common numerical schemes where space and time are treated independently (known as the method of lines), the time variable in space-time formulation is treated as another space variable. The discretized version of PDEs are then solved as boundary value problems in space-time domain. Several numerical examples will be presented.

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MS97

Lagrangian Particle Simulations of Geophysical Fluid Flow

This talk will describe recent Lagrangian particle simulations of geophysical fluid flow. We consider tracer transport and the barotropic vorticity equations on a rotating sphere. The numerical method is based on a Lagrangian form of the governing equations. The flow map is represented by moving particles that carry tracer and vorticity, and the particle velocity is recovered by the Biot-Savart integral. Adaptive refinement and remeshing techniques are used to resolve small scales and overcome particle distortion. We also hope to present preliminary results for the shallow water equations, where the particles also carry height and divergence.

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MS97

A High-Order Staggered Meshless Method for Stokes Equations with Applications to Electrokinetic Suspension Flow

Abstract Not Available at Time of Publication

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MS98

A Method for the Numerical Computation of Nonoscillatory Phase Functions

A large class of second order ordinary differential equations — including those defining the classical orthogonal polynomials, Bessel functions, the prolate spheroidal wave functions, and many other special functions — admit nonoscillatory phase functions. That is, phase functions which represent solutions using a quantity of information which does not depend on their frequency of oscillation. We will describe a robust numerical method for the calculation of nonoscillatory phase functions which requires only knowledge of the coefficients of the equation. We will also discuss several applications of phase functions, including the numerical computation of Gaussian quadrature formulas.

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MS98

Ultraspherical Spectral Method and Approximating Special Functions

The ultraspherical spectral method gives a fast algorithm for calculating solutions to differential equations to high accuracy. We explore its usage on special functions. By using suitable Jacobi-weighted variants, we can incorporate singularities in the solutions.

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MS98

Efficient Computation of Gaussian Quadrature Rules

We describe methods of computation of classical Gaussian quadrature rules (Hermite, Laguerre, Jacobi) which are effective both for small and large degree. The methods combine several evaluation schemes for the orthogonal polynomials involved together with the use of a globally convergent fourth order fixed point method for computing the nodes. The fast and certain convergence of the iterative method makes this an ideal approach for high precision computations.

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MS98

Computing Without Spherical Harmonics

Spherical harmonics expansions are a popular tool for accurate computations on spherical geometries that we intentionally avoid in this talk. Instead, we describe a whole collection of fast highly-adaptive algorithms for computing on the sphere based on the Fourier basis and the fast Fourier transform. Together with fast and well-conditioned spectral methods we are able to perform long-time Navier-Stokes simulations, model active biological fluids, and compute geophysical flows in spherical geometries.

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MS99

Asymptotic and Numerical Studies of Free Boundaries and Singular Shocks in Magnetized Target Fusion Reactors

Magnetized target fusion is a design for fusion energy that confines a plasma in a magnetic field and implodes it in a molten metal shell. To assess this design, we combine fluid dynamics of compressible fluids with free boundary problems, driven by external and plasma pressures; implement a finite volume scheme to perform a parameter sensitivity analysis; asymptotically estimate the plasma compression; and through studying a system with singular shocks, predict effects of asymmetric perturbations.

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MS99

Contagion Shocks in One Dimension

We consider an agent-based model of emotional contagion coupled with motion in one dimension that has recently been studied in the computer science community. The model involves movement with speed proportional to a fear' variable that undergoes a temporal consensus averaging with other nearby agents. We study the effect of Riemann initial data for this problem, leading to shock dynamics that are studied both within the agent-based model as well as in a continuum limit. We examine the model under distinguished limits as the characteristic contagion interaction distance and the interaction timescale both approach zero. Here, we observe a threshold for the interaction distance vs. interaction timescale that produces qualitatively different behavior for the system - in one case particle paths do not cross and there is a natural Eulerian limit involving nonlocal interactions and in the other case particle paths can cross and one may consider only a kinetic model in the continuum limit. Time permitting, we will also discuss recent extensions of the model to two dimensions.

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MS99

Singular Shocks in a Chromatography Model

We consider a system of two equations that can be used to describe nonlinear chromatography and produce a coherent explanation and description of the unbounded solutions (singular shocks) that appear in Mazzotti's model. We use the methods of Geometric Singular Perturbation Theory, to show existence of a viscous solution to Dafermos-DiPerna regularization.

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MS99

Particle-Laden Viscous Flow on An Incline: Singular Shock Solutions and Surface Tension Effects

We consider viscous suspensions on an incline containing particles. The lubrication model with surface tension is a system of mixed hyperbolic-parabolic type for the film height and particle concentration. The hyperbolic system exhibits exhibits singular shock solutions corresponding to accumulation of particles at the front. Surface tension regularizes these shocks and in two dimensions leads to fingering instabilities. We discuss some features of the model, present numerical simulations and compare to experimental results.

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MS100

Modeling the Dynamics of Immunological Memory to Malaria

Each year nearly 200 million people are infected with the malaria parasite. One of the most notable features of infection is the inability to acquire sterilizing immunity. Even with multiple exposures individuals remain semi-immune avoiding disease but not the parasite. We develop a mathematical model of the generation and maintenance of B cell and antibody response to malaria. We analyze simulated output to understand the origin of protective as well as ineffective immune responses in the presence of a multitude of varied proteins as well as antigenically varying proteins. We find that the level of persistent antibodies depends upon assumptions on the relative production of different type of antibody producing cells. Understanding the development and maintenance of protective immune responses to malaria is key in the on-going push towards elimination and eradication.

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MS100

Discontinuous Galerkin Methods for Boltzmann - Poisson Systems of Electronic Transport in Semiconductors

We will present in this talk a short survey the computational modeling of electron transport in semiconductors via Discontinuous Galerkin (DG) Methods for Boltzmann-Poisson (BP) kinetic models. We discuss the incorporation of anisotropic electronic band structures on DG deterministic solvers for BP, for modeling processes of transport and collision of electrons in semiconductors. We also address the computational modeling of reflection of electrons in a rough surface representing the physical boundary of the semiconductor via diffusive and general mixed reflection Boundary Conditions. Lastly, we present developments of positivity preserving DG schemes for Boltzmann - Poisson models in general curvilinear coordinates.

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MS100

Randomized Methods for Rank-Deficient Linear Systems

We present a simple, accurate method for solving consistent, rank-deficient linear systems, with or without additional rank-completing constraints. Such problems arise in a variety of applications, such as the computation of the eigenvectors of a matrix corresponding to a known eigenvalue. The method is based on elementary linear algebra combined with the observation that if the matrix is rank-k deficient, then a random rank-k perturbation yields a nonsingular matrix with probability close to 1.

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MS100

Polynomial Time Instance of the Maximum Weighted Co-2-Plex Problem

The maximum weighted co-2-plex problem (MWC2P) determines a subset of vertices of maximum total weight of a given graph, in which each vertex has degree at most one. We present a study of MWC2P for {claw, bull}-free graphs along with two polynomial time algorithms to solve it. The first algorithm transforms the given graph to solve an instance of the maximum weighted stable set problem utilizing Mintys algorithm. The second algorithm is an extension of Mintys algorithm and solves the problem in the original graph. Numerical results are provided to compare the aforementioned algorithms.

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MS101

The Miseducation of Data Scientists

In an age where information rules the day, those who are masterful in understanding and leveraging information lead the day. The recent significant rise in the number of programs offering Data Science degrees and courses begs the question if these programs are actually meeting the needs of the industry and what makes a Data Scientist a Data Scientist. We aim to define a framework around these questions to drive their education requirements.

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MS101

Strategies for Enabling Data Science Research and Education

In this talk we will demonstrate how real word data and programming languages can be used throughout an entire life-cycle of a graduate program in Data Science. In interdisciplinary fields, such as Data Science, the students often come from a variety of different backgrounds where, for example, some students may have strong mathematical training but less experience in programming. We will focus on the use of modern programming languages (e.g., Python) to improve students learning.

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MS101

Interdisciplinary Data Analytics - A Graduate Masters Degree Across Business, Engineering, and Science

We describe a fully interdisciplinary Data Analytics master degree program, executed through the cooperation of School of Business, School of Arts and Science, and School of Engineering, using faculty from all three backgrounds. The program core focus on developing a fundamental skill set that is then applied in a project based setting. The students have broad flexibility in initiating that project, typically with industry partners, that allows connecting that project to their background expertise and intended field of application.

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MS101

Education for Data Challenges in the 21th Century - BS/MS Program in Data Science at Umass

The emergence of massive data in wide domains poses big challenges to education in data science and analytics. In order to meet such challenges, we at the UMass Dartmouth has designed a curriculum which combines our understanding of the principle of data science, and our analysis of the current as well as the predicted future needs in data science. Our curriculum is comprehensive and flexible enough to meet data challenges of the 21st century.

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MS102

Elastic Fingering Pattern in a Hele-Shaw Cell

Experiments using two reacting fluids with the same viscosity in a Hele-Shaw cell show a gel-like phase can be produced at the interface. The interface surprisingly exhibits instabilities including fingering, fan-like patterns. We are interested in exploring the long-time, nonlinear interface dynamics using a boundary integral method, together with a rescaling scheme to dramatically speed up the intrinsically slow evolution of the interface. Numerical results reveal that there exist stable, self-similarly evolving morphologies.

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MS102

A Fast Platform for Simulating Flexible Fiber Suspensions Applied to Cell Mechanics

We present a novel platform for the large-scale simulation of fibrous structures immersed in a Stokesian fluid. We incorporate the key biophysical elements that determine the dynamics of cellular assemblies, which include the polymerization and depolymerization kinetics of fibers, their interactions with molecular motors and other objects, their flexibility, and hydrodynamic coupling. This work, to our knowledge, is the first technique to include many-body hydrodynamic interactions, and the resulting fluid flows, in cellular fiber assemblies.

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MS102

Accelerating Blood Simulations: a Coarse-Grained Theory to Understand Cellular Suspensions

The inhomogeneous concentration distribution of red blood cells and rigid particles normal to the flow direction is important in hemostasis, microfluidics and drug delivery. Realizing that whole blood simulation requires large-scale computation, we propose a coarse-grained theory to quantitatively understand cross-flow behaviors of particles in channel flow using fast small-scale simulations. We consider the effects of shear-induced diffusion and deformability-induced hydrodynamic lift at zero Reynolds number and compare our results to experiments and simulations.

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MS102

A High-Order Immersed Boundary Method for Solving Fluid Problems on Arbitrary Smooth Domains

We present a robust, flexible, and high-order Immersed Boundary method for solving the equations of fluid motion on domains with smooth boundaries using FFT-based spectral methods. The method retains much of the simplicity of the original Immersed Boundary method, and enables the use of simple implicit and implicit/explicit timestepping schemes to be used to solve a wide range of problems. We show results for the Stokes, Navier-Stokes, and Oldroyd-B equations.

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MS103

Generalized Multiscale Finite Element Method for Wave Propagation

In this talk, we present a new generalized multiscale finite element method for wave propagation in highly heterogeneous media. The method is based on some careful selections of basis functions on coarse grid elements. By using a suitable snapshot space and a local dimension reduction procedure, we obtain an efficient solver for the wave equation. We will present the analysis and some numerical results. The research is partially supported by Hong Kong RGC General Research Fund (Project: 400813).

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MS103

Automatic Smoothness Detection of the Resolvent Krylov Subspace Method for the Approximation of Semigroups

We will discuss rational Krylov subspace approximations to the matrix/operator exponential in semigroups. By comparing standard and rational Krylov methods with explicit and implicit time stepping methods, a motivation and explanation will be given why Krylov subspace methods might be more appealing than standard methods for the approximation of large operator/matrix functions that appear in time integration of evolution equations. Special emphasis will be given to the approximation of wave equations.

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MS103

Optimal Basis Computation for Multiscale Spectral Element Methods via Reduced Order Gramians

A critical component of spectral element and multiscale spectral methods is construction of localized basis functions that can approximate efficiently global full scale solutions. We consider propagative solutions of hyperbolic problems of limited bandwidth, for which we construct nearly (Nyquist rate) optimal approximation subspace via proper orthogonal decomposition (POD). The key to efficiency of our algorithm is matrix-rational approximation of

the frequency-limited Gramian and consecutive application of the Lanczos algorithm.

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MS103

On Rational Krylov Subspace Methods for Large-Scale Time and Frequency-Domain Wavefield Computations

Krylov subspace techniques are widely used in many application areas ranging from model-order reduction of dynamical systems to diffusive PDEs. In this talk we show the effectiveness of rational Krylov subspaces for hyperbolic wavefield problems. Numerical experiments illustrating the performance and limitations of such algorithms are discussed along with possible physics-based modifications that speed up their convergence. A comparison between rational and polynomial/extended Krylov subspace techniques is included as well.

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MS104

Applications of the Static Condensation Reduced Basis Element Method to Industrial Problems

The Static Condensation Reduced Basis Element (SCRBE) method enables component-based and parameterized reduced order models of large-scale systems. This methodology is well-suited to industrial problems, e.g. to provide Digital Twins of large-scale infrastructure. In this talk, we give an overview of the key ideas of the SCRBE method, and then present a series of applications to real-world problems which have been implemented by Akselos.

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MS104

PDE Apps for Simulation; Application to Elasticity and Acoustics

Parametrized PDE apps are PDE solvers which satisfy stringent per-query performance requirements dictated by the human attention span. PDE apps are relevant in many-query interactive contexts such as design and education. Our approach comprises four ingredients: component-to-system synthesis, formulated as static condensation; reduced basis approximation, informed by evanescence and low-dimensional parametric manifolds; offline-online computational decomposition; cloud-based parallelization. We demonstrate several applications in elasticity and acoustics.

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MS104

Fully Certified, Adaptive and Localized Reduced Basis Methods

We present recent advances in the context of the localized reduced basis multi-scale method for parametric elliptic multi-scale problems with possibly heterogeneous diffusion coefficients [M. Ohlberger and F. Schindler, *Error Control for the Localized Reduced Basis Multiscale Method with Adaptive On-Line Enrichment*, SIAM J. Sci. Comput., 2015, 37, A2865-A2895], in particular regarding fully adaptive basis enrichment based on a novel localized a posteriori error estimate on the full approximation error.

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MS104

A Multiscale Reduced Basis Method for Wave Propagation in Heterogeneous Materials

We present a model and variance reduction method for computing statistical outputs of stochastic wave propagation problems through heterogeneous materials. We combine the multiscale continuous Galerkin (MSCG) discretization and the reduced basis method for the Helmholtz equation with a multilevel variance reduction strategy, exploiting the statistical correlation among the MSCG and reduced basis approximations to accelerate the convergence of Monte Carlo simulations. We analyze the effect of manufacturing errors on waveguiding through photonic crystal structures.

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MS105

Numerical Methods for Adaptive Shallow Water Equations in Coastal Ocean Modeling

Shallow water approximation to coastal ocean dynamics is commonly applied for studying tidal waves, storm surges and tsunami inundation. Robust numerical implementations allow taking account for the complex geometry of coastal areas. The problem setting requires representing a large span of spatial and sometimes temporal scales, ranging from a few meters of resolution for representing reefs and other near-shore features up to several hundreds of kilometers to include tidal wave behavior. Thus, multiscale robust numerical schemes need to be found for accurate coastal ocean modeling, and a brief overview of approaches will be given in this presentation.

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MS105

Wave Amplification and Its Impact on Onshore Mass Transport

The geomorphological expression of storm surge events can have a severe impact on the population and the environment in coastal areas. In order to study the relationship between ocean wave energy and onshore mass transport, we investigate the effect of uneven submarine topography on wave amplification with a higher order spectral method that solves Euler equations. Numerical simulations show an up to sixfold amplification of ocean waves and their potential to move large structures inland.

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MS105

Two-Layer Wind-Wave Coastal Ocean Models

In this talk, we present the development of an accurate, yet efficient, multiscale wind-wave model. A key component of the investigation is an exploration into the interplay of the short-crested gravity waves with that of the long crested currents, particularly in the context of the two layer shallow water equations. Numerical results illustrate the models capability to generate, propagate, and dissipate short-crested gravity waves in a variety of coastal environments.

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MS105

A Class of Mimetic Ocean Primitive Equation Models

We describe the mimetic discretization of ICON-O, a new general circulation model on a icosahedral spherical C-grid. The models dynamical core as well as its oceanic parametrizations use a coherent mimetic discretization that allow an energetic consistent change of grid geometry and of reconstructions. This leads to a whole class of energetic consistent models. A sequence of simulations is presented that range from idealized experiments to eddy-resolving global ocean simulations.

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MS106

The Inverse FMM as a Preconditioner for Dense Linear Systems

In this talk, we present the inverse fast multipole method as an approximate fast direct solver for dense linear systems, with a computational cost scaling linearly with the problem size. The method can be used as a stand-alone direct solver or as a preconditioner in an iterative method. We use low-rank approximations to represent well- separated interactions; this is done in a multi-level fashion. Applications related to mesh deformation, Stokes flow, and acoustics are discussed.

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MS106

Fast Direct Solvers as Preconditioners for Evolved Geometries

Problems involving evolving geometries such as Stokes' flow or shape optimization require many solves a large number of geometries. Typically, iterative solution techniques requiring many iterations are used as the cost of constructing a direct solver is too expensive to be done for each new geometry. This talk illustrates the potential of creating a direct solver for a reference geometry via a fast method and using it as a preconditioner for the evolved geometries.

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MS106

On the Use of Low Rank Approximations for Sparse Direct Solvers

In this talk, we describe a preliminary fast direct solver using HODLR library to compress large blocks appearing in the symbolic structure of the PaStiX sparse direct solver. We will present our general strategy before analyzing the practical gains in terms of memory and floating point operations with respect to a theoretical study of the problem. Finally, we will discuss the impact of reordering technic to enhance the low-rank compression.

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MS106

Structured Eigenvalue Approximation and Accuracy

We study how to approximate the eigenvalues of some structured matrices as well as more general cases. The approximation accuracy is closely related to the rank structured compression, which gives us flexibility to control the efficiency and effectiveness. In particular, we also show that a low-accuracy structured approximation can already give satisfactory estimations of the locations of the eigenvalues. This is then particularly useful for preconditioning. This is joint work with James Vogel and Xin Ye.

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MS107

WENO-based Line Transpose Approach for Vlasov Equation

We will present a high order implicit Method of Line Transpose (MOLT) method based on a weighted essentially non-oscillatory (WENO) methodology is developed for one-dimensional linear transport equations and further applied to the Vlasov-Poisson (VP) simulations via dimensional splitting. In the MOLT framework, the time variable is first discretized by a diagonally implicit strong-stability-preserving Runge-Kutta method, resulting in a boundary value problem (BVP) at the discrete time levels. Then an integral formulation coupled with a high order WENO methodology is employed to solve the BVP. As a result, the proposed scheme is high order accurate in both space and time and free of oscillations even though the solution is discontinuous or has sharp gradients. Moreover, the scheme is able to take larger time step evolution compared with an explicit MOL WENO scheme with the same order of accuracy. We perform numerical experiments on several benchmarks including linear advection, solid body rotation problem; and on the Landau damping, two-stream instabilities, and bump-on-tail by solving the VP system. The efficacy and efficiency of the proposed scheme is numerically verified.

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MS107

Constraint-Preserving High Order Schemes by Lagrangian Multipliers

We propose a high order method with Lagrangian multiplier to preserve the divergence-free constraint in a Vlasov-Maxwell system.

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MS107

Runge-Kutta Discontinuous Galerkin Method with a Simple and Compact Hermit Weno Limiter

We design compact limiters using weighted essentially non-oscillatory(WENO) methodology for DG methods solving hyperbolic conservation laws, with the goal of obtaining a robust and high order limiting procedure to simultaneously achieve uniform high order accuracy and sharp, non-oscillatory shocktransitions. The main advantage of these compact limiters is their simplicity in implementation, especially on multi-dimensional unstructured meshes.

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MS108

Making Big Data Systems Efficient and Easy to Program

Since its inception, virtual memory has become a powerful and ubiquitous abstraction for allocating and managing memory with a flexible and clean programming model. Typically, the systems community has been comfortable paying a performance tax for these programmability benefits. Unfortunately, emerging software with large data requirements (e.g., large graphs, key value stores, virtualization), and emerging hardware (e.g., GPUs) requiring manual data orchestration, which increases this performance tax drastically, while also losing programmability benefits. In this talk, I discuss techniques to reclaim this lost performance and programmability by enriching existing address translation hardware to more elasticity adapt to memory allocation aspects of the operating system. Specifically, I show how hardware support that detects patterns in page table allocation can be used to design high performance address translation hardware. In addition, I discuss how to design memory management units for accelerators in support of unified address spaces.

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MS108

Databases and Mathematics for Big Data

Over the past decade, there have been some major shifts in the technologies being used to store and index large quantities of scientific data. The latest trend has been towards a polystore and/or federated database solutions. In this talk, I will discuss BigDAWG, a suite of technologies we are developing to address the polystore or federated database challenge. I will also discuss how mathematical foundations play a part in solving the problem of data management.

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MS108

Fast Processing of Large Graph Applications Using Asynchronous Architectures

Graph algorithms and graph processing are at the core of many computation problems, from social graphs (Facebook, LinkedIn, Twitter, etc.) to location graphs (map, power grid, telephone network, etc.). Yet, computing on large graphs remains extremely difficult. In graph-based applications, memory access patterns often lack locality. In this work, we develop a scalable graph processor that computes directly on the graph structure of the algorithm or application without intermediate representations, e.g., sparse matrix representation. The processor has a large number of interconnect processing elements. Each processing element represents a graph node or a set of nodes. The processing elements are asynchronous with ready signal for data communications. Our preliminary results show 2.4x improvement over the algebraic transformation approach.

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MS108

Role of Scientific Computing in Gas Turbine Engine Design

Performance of modern gas turbines for propulsion and power generation is closely tied to lower pollutant emissions, higher fuel efficiency, and better durability. These objectives are often conflicting and require considerable improvements to design and sustain growth. In the past decade, industry has been driving the application of simulation technologies to guide design of modern gas turbines. This talk highlights the impact of scientific computing and data analytics on gas turbine combustor design.

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MS109

Multigrid Reduction in Time, Theory and Applications

In this talk, we will present theoretical results regarding the convergence of the two level multigrid reduction in time (MGRIT) algorithm. We consider the application of the method to a set of explicit and implicit Runge-Kutta schemes and characterize its behavior for linear problems. We illustrate the MGRIT algorithm and the theoretical results with various applications such as transient advection and diffusion, confirming our analysis. LLNL-ABS-681700

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MS109

Assessing Time Parallel Efficiency for Test Problems in Climate Science

We will describe ongoing efforts to evaluate the effectiveness of the Parallel Full Approximation Scheme in Space and Time (PFASST) on a suite of test problems inspired by geophysical flows and climate models. The relative merits of implicit versus explicit higher-order time stepping and the effect of diffusion on the convergence of PFASST will also be discussed.

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MS109

Analysis of a Fully Scalable Balanced Parareal Method

Abstract Not Available at Time of Publication

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MS109

Fault-Tolerant Parallel-in-Time Integration with PFASST

For time-dependent PDEs, parallel-in-time integration with e.g. the "parallel full approximation scheme in space and time" (PFASST) is a promising way to accelerate existing space-parallel approaches beyond their scaling limits. In addition, the iterative, multi-level nature of PFASST can be exploited to recover from hardware failures, preventing a breakdown of the time integration process. In this talk, we present various recovery strategies, show their impact and discuss challenges for the implementation on HPC architectures.

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MS110

Nonlinear Price Impact and Portfolio Choice

In a market with price-impact proportional to a power of the order flow, we derive optimal trading policies and their implied welfare for long-term investors with constant relative risk aversion, who trade one safe asset and one risky asset that follows geometric Brownian motion. These quantities admit asymptotic explicit formulas up to a structural constant that depends only on the price-impact exponent. The model nests the square-root impact law, linear impact, and proportional transaction costs.

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MS110

A Second-Order Expansion of the Value Function in the Problem of Optimal Investment in Incomplete Markets

In the framework of incomplete financial market where the stock price dynamics is modeled by a continuous semimartingale, an explicit quadratic expansion for the power investor's value function and a first-order expansion for the corresponding optimal wealth process - seen as a function of the underlying market price of risk process - are provided. An example illustrating the result is also given. The talk is based on the joint work with Kasper Larsen, Mihai Sirbu, and Gordan Zitkovic.

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MS110

The Systemic Effects of Benchmarking

We show that the competitive pressure to beat a benchmark may induce institutional trading behavior that exposes retail investors to tail risk. In our model, institutional investors are different from a retail investor because they derive higher utility when their benchmark outperforms. This forces institutional investors to take on leverage to overinvest in the benchmark. Institutional investors execute fire sales when the benchmark experiences shock. This behavior increases market volatility, raising the tail risk exposure of the retail investor. Ex post, tail risk is only short lived. All investors survive in the long run under standard conditions, and the most patient investor dominates. Ex ante, however, benchmarking is welfare reducing for the retail investor, and beneficial only to the impatient institutional investor.

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MS110

Market Stability and Indifference Prices

Consider a derivative security whose underlying is not replicable yet is highly correlated with a traded asset. As the correlation between the underlying and traded asset increases to 1, do the claim's indifference prices converge to the arbitrage-free price? In this talk, I will first present a counterexample in a Brownian setting with a power utility investor where the indifference prices do not converge. The counterexample's degeneracies are alleviated for utility functions on the real line, and a positive convergence result will be presented in this case.

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MS111

Chordal Structure and Polynomial Systems

Chordality and bounded treewidth allow for efficient computation in linear algebra, graphical models, constraint satisfaction, and many other areas. We analyze to what extent chordality might help in computational algebraic geometry. To this end, we propose new techniques for solving polynomial equations. By maintaining graphical structure, our methods can outperform standard algorithms in many cases. Besides the theoretical developments, we illustrate the suitability of our methods in examples from graph colorings, cryptography and sensor localization.

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MS111

Hilbert's Nullstellensatz and Perfect Matchings

There are many elegant and compact modelings of NP-complete combinatorial problems as systems of polynomial equations that yield exponential size Hilberts Nullstellensatz certificates of infeasibility. Similarly, there are combinatorial problems known to be in P that yield simple certificates of fixed-degree. In this project, we explore the perfect matching problem (well-known to be P), and surprisingly demonstrate encodings where the certificates of infeasibility are exponential-size.

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MS111

Symmetric Polynomials from Extremal Combinatorics

Many problems in extremal combinatorics boil down to certifying the non-negativity of a symmetric polynomial. Razborov's flag algebras provide a powerful method for doing this. We show that these polynomials can also be certified using standard symmetry reduction techniques from semidefinite programming. The SDPs that need to be solved have constant size even though the number of variables in the polynomial is going to infinity.

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MS111

The Ubiquity of Determinantal Equations

I will discuss how and why, from the point of view of geometry, equations involving determinants, or more generally minors of matrices, are nearly universal, and then sketch some work that is intended to improve our ability to manipulate such equations.

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MS112

High Performance Multi-Level Covariance Estimation and Kriging for Large Scale Non-Gridded Spatial Datasets

In this talk we introduce techniques from Computational Applied Mathematics and High Performance Computing to efficiently estimate the covariance function parameters and compute the best unbiased predictor. We develop a multi-level approach that produces a new set of contrasts. The first advantage is that the covariance parameters are decoupled from the deterministic trend thus the parameter estimation problem can be solved independently from the trend. In addition, the covariance matrix of the new contrasts exhibits fast decay and is better conditioned than the original covariance matrix. We demonstrate our approach on problems of up to 512,000 observations with a Matérn covariance function and highly irregular placements of the observations. These test examples are numerically unstable and hard to solve with traditional methods.

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MS112

Bayesian Optimization with a Finite Budget: An Approximate Dynamic Programming Approach

We reformulate Bayesian optimization with finite budget as a dynamic programming instance. This results in a complex problem with uncountable, dimension-increasing state space and uncountable control space. We examine two classical techniques to solve the approximate dynamic programming problem: certainty equivalent control, and rollout. We prove that certainty equivalent control reduces to a suboptimal, over-exploiting optimization policy. The performance of rollout is examined numerically and is shown to outperform the popular efficient global optimization policy.

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MS112

Mixture of Experts with Kriging: A Divide-and-Conquer Approach to Model Heterogeneous Function Profiles

Kriging construction requires finding a set of hyperparameters that best fit the function to be approximated. The local approximation accuracy is therefore compromised when modeling a heterogeneous function profile. To address this issue, a mixture of experts approach is developed based on the divide-and-conquer strategy, by constructing several local kriging models and determining the optimum hyperparameters locally. A probabilistic approach is adopted to partition the input space and combine the local predictions. The efficiency and accuracy of this approach are demonstrated in the context of aerodynamic performance prediction problem.

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MS112

Speeding Up Kriging by Using Pivoted Cholesky Decomposition and Low-Rank Structures

Kriging is often impaired in terms of costs and accuracy by ill-conditioned covariance matrices of large dimension N. We propose to tackle both of these problem by using a pivoted Cholesky decomposition (PCD) and a rank-k formulation of Kriging. The PCD solves a rank-deficient but consistent system. By reformulating the maximum likelihood training accordingly, the complexity is reduced to $\mathcal{O}(k^2N)$ with $k \ll N$. In numerical tests our approach displays an accuracy comparable to regularization approaches.

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MS113

Inverse Medium Scattering with Multiple Frequency Data and Multiple Angles of Incidence

We consider the problem of reconstructing the medium from scattering measurements. The input data is assumed to be the far-field generated when a plane wave impinges on an unknown medium from multiple directions and at multiple frequencies. It is well known that this inverse scattering problem is both ill posed and nonlinear. We will use the recursive linearization algorithm of Chen to turn this problem in a sequence of well-posed problems. During the course of solving the inverse problem, we need to compute the solution to a large number of forward scattering problems. For this, we use high-order accurate PDE solver coupled with a fast direct solver.

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MS113

High-Performance Surface Integral Equation Solvers Towards Extreme-Scale Electromagnetic Computation

This work investigates an adaptive, parallel and scalable integral equation solver for extreme large multi-scale electromagnetic computing. A complicated surface model is decomposed into a collection of components, which are discretized independently and concurrently using a discontinuous Galerkin boundary element method. An additive Schwarz domain decomposition method is employed for the efficient and robust solution of linear systems resulting from discontinuous Galerkin discretizations. The work leads to rapidly-convergent integral equation solvers for large multi-scale objects.

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MS113

A Tensor-Train Accelerated Solver for Integral Equations in Complex Geometries

We present a framework using the Tensor Train decomposition to accurately and efficiently solve volume and boundary integral equations in three dimensions. We describe how the Tensor-Train decomposition can be used as a hierarchical compression and inversion scheme for matrices arising from the discretization of integral equations. For a broad range of problems, computational and storage costs of the scheme are $O(\log N)$ and the invesrse can be applied in $O(N \log N)$.

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MS113

Voxelized Geometries, Volume Integral Equations, and the Reemergence of FFT-Based Sparsification

In disciplines as diverse as microfluidics, nanotechnology, medical imaging, and 3-D printing, model generation must be completely automatic, yet extremely reliable. This combination has favored model generation based on the most-easily-manipulated geometric element, the cube. When volume integral equations are used to analyze cube-based models (referred to as pixelized" in 2-D and voxelized" in 3-D), the result is often a multidimensional Toeplitz-plus-Hankel (TPH) matrix, well-known to be easily sparsified with the FFT. In this talk we will describe several recent applications of volume integral equations applied to voxelized models, and describe some of the newer challenges and insights, such as using numerically-computed TPH approximations to non-TPH problems.

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MS114

Bayesian Fused Lasso Regression for Dynamic Binary Networks

We propose a multinomial logistic regression model for link prediction in a time series of directed binary networks. To account for the dynamic nature of the data we employ a dynamic model for the model parameters that is strongly connected with the fused lasso penalty. In addition to promoting sparseness, this prior allows us to explore the presence of change points in the structure of the network. We introduce fast computational algorithms for estimation and prediction using both optimization and Bayesian approaches. The performance of the model is illustrated using both simulated and real data from a financial trading network in the NYMEX natural gas futures market.

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MS114

Measure-Theoretic Augmentation of Multifidelity

Monte-Carlo Estimation

Estimating the statistics of high fidelity computational models requires the integration of a model and a probability density. When the model is complex, a sample-based integration method such as Monte Carlo or Quasi-Monte Carlo may be the only feasible approach. Unfortunately, convergence for these methods is slow. We exploit surrogate models to reduce computational cost by using multi-fidelity Monte-Carlo estimation. We augment convergence rates with techniques obtained from the measure-theoretic interpretation of sample-based integration algorithms.

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MS114

Stochastic Characteristics of Quantum-Inspired and Quantum Algorithms

Our ongoing work focuses on algorithms related to quantum computing. We focus on algorithms which are either (1) "inspired" by quantum mechanical constructs but designed for implementation on classical/conventional hardware or (2) designed for implementation on quantum hardware. We provide an overview of stochastic aspects of these algorithms and of typical systems which they might be used to model. We demonstrate how we have considered these aspects in designing software for quantum-inspired algorithms.

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MS114

Estimating $\mathcal{R}_0$ For Avian Influenza Through Transmission Chains And Data Fitting

The transmission of avian influenza between humans is extremely rare, and it mostly affects individuals who are in contact with infected poultry. Although this scenario is uncommon, there have been multiple outbreaks that occur in small infection clusters in Asia with relatively low transmissibility, and thus are too weak to cause an epidemic. Still, sub-critical transmission from stuttering chain data is vital for determining whether avian influenza is close to the threshold of $\mathcal{R}_0 > 1$. In this talk, we will explore two methods of calculating $\mathcal{R}_0$ using transmission chains and parameter estimation.

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MS115

Viscous Singular Shock Profiles for a System Modeling Incompressible Two-Phase Fluid Flow

We consider the Dafermos regularization $u_t+f(u)_x = \epsilon t u_{xx}$ for a system of conservation laws modeling incompressible two-phase flow in one space dimension. Using Geometric Singular Perturbation Theory, we prove the existence and weak convergence of viscous singular shock profiles. We also show that the maximum of the viscous solution is of order $\exp(\epsilon^{-1})$.

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MS115

Two-Species Chromatography with Anti-Langmuir Isotherms: A Case Study for Singular Shocks

The PDE for two-component chromatography with the Langmuir isotherm (a standard approximation) form a system of hyperbolic conservation laws. A decade ago, Marco Mazzotti developed a model similar to the Langmuir isotherm, but with a change of sign. The formulas for constructing Riemann solutions break down, and numerical simulation suggested that singular shocks appeared. We examine the mathematical structure of these singular shocks, using Geometric Singular Perturbation Theory. Our results shed light on the behavior of the chemical system and advance the mathematical theory of singular shocks.

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MS115

Singular Shocks in Nonlinear Chromatography: Theoretical and Experimental Considerations

We study the system

$$(u_i + v_i)_\tau + (u_i)_x = 0 \quad (i = 1, 2) \tag{3}$$

with

$$v_i = \frac{a_i u_i}{1 - u_1 + u_2} \quad (i = 1, 2). \tag{4}$$

These conservation equations are of interest in nonlinear chromatography, where u_i and v_i are the dimensionless liquid and adsorbed phase concentrations of species i, respectively. Under certain conditions, solutions to this system exhibit singular shocks (Mazzotti, *Ind. Eng. Chem. Res.*, 2009, 48(16):7733-52). Properties of these singularities are derived and confirmed by three different methods, based on smooth approximations, on box approximations, and on Colombeau generalized functions. Furthermore, we provide an overview of experimental results and of challenges regarding their experimental evidence (Jermann et al., *J. Chrom. A*, 2015, 1425:116-28).

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MS115

Shock Waves in the Presence of Dispersion

Dispersive shock waves (DSW) of the KdV equation have a well-defined structure that includes a modulated periodic wave train, led by a solitary wave. This structure is also seen in the modified KdV equation,

$$u_t + (u^3)_x = \mu u_{xxx}, \tag{5}$$

in which the flux $f(u) = u^3$ is non-convex. However, there is a richer set of DSW for equation 5, including contact DSW (if $\mu < 0$) and kinks (if $\mu > 0$). It is also instructive to compare solutions of (5) with those of the modified KdV-Burgers equation, which includes a diffusive term,

$$u_t + (u^3)_x = \nu u_{xx} + \mu u_{xxx}, \quad \nu > 0. \tag{6}$$

The structure of shock waves for (6) is quite different, and fits the classical conservation laws description of Lax and Oleinik if $\mu < 0$. However, for $\mu > 0$, there are undercompressive shocks, which are diffusive equivalents of the kink solutions of 5. Finally, I describe stationary shock solutions of the BBM equation

$$u_t + uu_x = \mu u_{xxt}, \tag{7}$$

and of a version of the Boussinesq equations of shallow water flow. I show that smooth initial data approximating an expansion shock persists in time, weakening to give way to a rarefaction wave only algebraically in time.

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MS116

Shaping A Well-Rounded Analyst

Becoming a successful data analyst requires more than a basic mathematics or statistics degree. It relies on ingenuity, a solid computer science foundation, and strong communication skills at a business level. Industry questions and data do not fit a standard mold. As an industry representative I discuss how to step outside of the textbook and into real-world scenarios to provide students with every advantage to succeed.

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MS116

Mathematics and Computer Science: Education in Data Science, Data Engineering and Data Analytics at Tum

Data Science plays an important role in different areas like Computer Science, Mathematics and Probability Theory, Ethics, and all kind of applications in Economy, Medicine, Geoscience and more. Therefore, at the TUM these different educational programs will be combined into an integrated study program that connects Data Science master programs from different faculties in order to harmonize the various courses and allow a broad spectrum of different study paths. This comprises mutual exchange of lectures, common projects, and a joint panel that coordinates the different programs. In this talk we will describe this approach.

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MS116

Motivating Data Science students with Hackathons and Oi-X

Mid 2013 the study profile Data Science/Big Data was launched at the Technical University of Denmark. This was a partial result of a sector development project on the uses of Big Data. In order to create and also sustain awareness of the study profile among students and industry a number of different instruments are used ranging from company presentations on use of data science in their area to 48 hour hackathons and open innovation-X events.

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MS116

Data Science: A Natural Fit in the Liberal Arts Curriculum

In Fall 2015, the joint Department of Mathematics, Statistics, and Computer Science at Macalester College began to offer a minor in data science. We will discuss the role of data science in the liberal arts curriculum, how this new program fits with Macalesters strategic plan, and the requirements of the minor. We will also reflect on hurdles faced during the minor approval process and plans for building a pervasive culture of data science across campus.

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MS117

Convergence of a Boundary Integral Method for 3D Interfacial Flow with Surface Tension

We consider interfacial Darcy flow with surface tension in 3D; for such a flow, a fully explicit method would face a third-order stiffness constraint. For such flows in 2D, Hou, Lowengrub, and Shelley (HLS) removed the stiffness by devising a semi-implicit timestepping scheme. Subsequently, Ambrose and Masmoudi extended the ideas from the HLS scheme to well-posedness proofs of initial value problems for interfacial flows in 2D and in 3D. We will describe a semi-implicit scheme which removes the stiffness from 3D interfacial Darcy flow with surface tension, which is in turn influenced by these analytical works. We furthermore are able to prove that a version of this method converges. The main step in the convergence proof is establishing energy estimates for stability, which are closely related to the prior energy estimates for well-posedness. This includes joint work with Yang Liu, Michael Siegel, and Svetlana Tlupova.

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MS117

Low Resolution Simulations of 2D Vesicle Suspensions

Vesicle suspensions serve as experimental and numerical proxies for red blood cells. Their simulation poses numerical challenges such as non-local interactions, a local inextensibility constraint, and stiff governing equations. Algorithms such as time adaptivity, anti-aliasing, surface reparameterization, and local corrections to the vesicle shape must be used to maintain stability at low resolutions for long time horizons. We will closely look at how effective the low-resolution simulations can capture the true physics of vesicle flows.

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MS117

A Fast Algorithm for Particulate Flows Through Complex Periodic Geometries

We present a new periodization algorithm that, unlike classical boundary integral equation methods, does not rely on periodic Greens functions. Instead, it combines the free-space Greens function with a small auxiliary basis and imposes periodicity as an extra linear condition. Incorporating stable time-marching schemes and fast algorithms, we were able to simulate the hydrodynamics of over 1000 deformable particles flowing through a periodic microfluidic-chip geometry in less than a minute per time-step on a laptop..

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MS117

On the Gating of a Mechanosensitive Channel by Fluid Shear Stress

Mechanosensation is important in biological fluid-structure interaction. To understand the biophysics of mechanosensation, we use smoothed dissipative particle dynamics (SDPD) to simulate vesicle/cell in three types of flow, and calculate the dynamic membrane tension. In combination with a simple continuum model for a mechanosensitive (MS) channel, SDPD simulation results reveal shearing adhered vesicles/cells is more effective to induce membrane tension sufficient to stretch MS channels open than a free shear flow or a constrictive channel flow.

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MS118

Nested Krylov Methods for Solving the Time-Harmonic Elastic Wave Equation at Multiple Frequencies

Recently we proposed an iterative framework for the solution of shifted systems that uses an inner multi-shift Krylov method as a preconditioner within a flexible outer Krylov method by exploiting collinear residuals. In this talk, we explain the relation of our approach with Rational Krylov Methods. We will show how the time-harmonic elastic wave equation at multiple frequencies can be formulated as a sequence of shifted systems and we will illustrate the performance our solution method on such problems.

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MS118

Optimizing Radiation Boundary Conditions and Absorbing Layers for Time Domain Problems

Accurate approximate radiation boundary conditions are essential for most time-domain simulations of waves. For models equivalent to the scalar wave equation in the far field, optimal local conditions based on rational approximations to the DtN map can be constructed. However, for more complex systems, such as those arising in elasticity, optimal conditions and their complexity are not directly known. Here we describe our efforts to numerically construct accurate conditions for arbitrary hyperbolic systems.

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MS118

Multi-Scale Mimetic Reduced-Order Models for Large-Scale Wavefield Simulations

We have developed novel approach for discretizing spatial operator in wavefield simulations. We split the reference fine grid model into multiple subdomains. The adjacent subdomains are conjugated using Neumann-to-Dirichlet map. We construct sparse reduced-order model of NtD map for each cell via transformation to Stieltjes continued fraction. This method perfectly fits high performance computing platforms and allows to simulate wavefields in media with unlimited complexity and to achieve spectral accuracy even on regular model-independent grid

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MS118

Asymptotically Corrected Krylov Subspace Model-Order Reduction of Wavefields in Travel-Time Dominated Structures

In this talk we present travel time or asymptotically corrected Krylov subspace methods to efficiently compute time- and frequency-domain wavefields in inhomogeneous structures. Fields characterized by large travel times can be effectively captured, by adding travel time information to parameter dependent Rational Krylov subspaces. This method provides reduced-order models of small order, which can be incorporated in wavefield inversion schemes. Numerical experiments will be presented that illustrate the performance of the method.

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MS119

Advances in Reduced Order Methods for Computational Fluid Dynamics

We present some recent advances in reduced order methods for parametrized problems in computational fluid-dynamics. We focus our attention on stability of flows, multi-physics, like fluid-structure interaction or porous media, domain decomposition and optimal control. These topics are crucial in order to be able to deal efficiently, from the computational point of view, with more and more complex fluid-mechanics problems, characterized by several parameters, extended domains, and higher Reynolds numbers.

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MS119

Large Eddy Simulation Reduced Order Models

This talk proposes several large eddy simulation reduced order models (LES-ROMs) based on the proper orthogonal decomposition (POD). Explicit POD spatial filtering is introduced and used to increase fidelity in calculations of large structures present in the ROM. These explicit POD spatial filters allow the development of two types of ROM closure models: phenomenological and approximate deconvolution. The new LES-ROMs are tested in the numerical simulation of a three-dimensional flow past a circular cylinder.

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MS119

Simultaneous Spatio-Parameter Adaptivity for Parametrized Problems in CFD

We develop a reliable model reduction approach for parametrized PDEs in fluid mechanics. The key ingredients are a goal-oriented a posteriori error estimate for engineering quantities of interest, anisotropic mesh adaptivity that resolves solution features over a wide range of spatial scales, and a localized model reduction technique which empirically identifies low-dimensional spaces adapted to the parametric manifold. We demonstrate the approach for the compressible Navier Stokes equations in aerodynamics.

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MS119

Goal-Oriented Model Order Reduction for Vector-Valued Variables of Interest

We focus on the estimation of vector-valued variables of interest (VoI) associated to parameter-dependent equations using projection-based model order reduction methods. After extending the classical primal-dual method for vector-valued VoI, we introduce a new approach based on a saddle-point formulation. Both methods involve three reduced spaces: the approximation space and the test space associated to the primal variable, and the approximation space for the dual variable. In the spirit of the Reduced Basis method, we propose greedy algorithms for the construction of these reduced spaces.

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MS120

Scaling Element-Based Galerkin Methods on Multi-core and Many-Core Computers for Geophysical Fluid Dynamics Models

Element based Galerkin (EBG) methods are well suited for Geophysical Fluid Dynamics simulations on both multi-core and many-core clusters. This stemming from the fact that most operations in EBG methods are local in nature. This talk will focus on scalability of the Non-hydrostatic Unified Model of the Atmosphere (NUMA) on various super-computers consisting of CPUs, GPUs, Xeon-Phi and other accelerators. NUMA solves the shallow water equations and the Euler equations using a unified continuous / discontinuous Galerkin framework. We believe the use of these high-order EBG methods for discretization will improve scalability in other Geophysical Fluid Dynamics applications as well. To ensure scalability on future exa-scale supercomputers, one also needs to target heterogeneous architecture. We use device-agnostic programming techniques for portability and ensuring best performance for each device in the system. We were able to achieve a strong scaling efficiency of about 99% using 3-million MPI ranks on the MIRA supercomputer which consists of only CPUs. The GPU version achieved two orders of magnitude speedup over the CPU version, while maintaining a 90% weak scaling efficiency using up to 16384 GPUs of the titan supercomputer. In this talk, we will discuss the methods and optimization used to achieve the excellent scalability on both multi- and many-core machines.

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MS120

Applications of Tsunami Inundation Models in the North of Chile

The city of Arica, in the north of Chile, has been affected by tsunami inundation several time in his recent history. In the 1868 magnitude 9.0 Arica event the U.S. Navy ship "Wateree" was transported 300 meters inland. This area has been identify with a seismic gap and therefore potential big events are expected. Using an unstructured finite volume scheme we simulate different potential tsunami inundation scenarios and extract conclusions regarding hazard zones.

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MS120

Adjoint Error Estimation for Tsunami Modeling

The GeoClaw software uses block-structured adaptive mesh refinement to selectively refine around propagating waves and/or coastal regions of interest. Because of multiple reflections or edge waves it can be difficult to determine what waves need to be refined. Using a Richardson extrapolation error estimator to estimate the point-wise error in the solution and then using the adjoint solution to estimate its effect on the location of interest enables more precise and efficient refinement.

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MS120

Improved Multi-Scale Characterization of Hurricane Storm Surge

We present results of novel characterizations that explore the characterization of multiscale hurricane storm surge destructive forces on highly populated areas. The potential damage impact of impending hurricanes in the United States has traditionally been measured by the

Saffir-Simpson scale, a simple model to provide weather forecasters and emergency planners with a Category 1-5 rating. However, reliance on this scale as an indicator of storm surge, the primary destructive force during a hurricane, leads to misconceptions by the public and scientists alike of the impending danger. This simple technique does not rely on the numerous scales and environmental factors imperative to the characterization of an impending hurricane. In this talk, it is shown that the size of a hurricane windfield, the intensity, and a newly proposed potential kinetic energy are much more influential/indicative of resulting storm surge and related flooding. We present results of a suite of synthetic storms impacting the Galveston Bay, Texas area that demonstrates this phenomena. High performance computing simulations are performed on the Texas Advanced Computing Centers supercomputers using the highly accurate and robust Advanced Circulation (ADCIRC) numerical model.

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MS121

Fast Solvers for 3D elastodynamic Boundary Element Methods

In traditional Boundary Element Methods (BEM), the dimensional advantage is offset by the fully-populated nature of the matrix. The Fast Multipole accelerated BEM (FM-BEM) permits to speed up the solution. In 3D elastodynamics, the method is efficient but the number of iterations can significantly hinder the overall efficiency. Using the H-matrix arithmetic and low-rank approximations, we derive a fast LU solver to precondition the FM-BEM. The efficiency to study elastic wave propagation problems is shown.

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MS121

FMM Pre-Conditioners for Highly Ill-Conditioned Structured Matrices in Approximation Theory

We have recently proposed a minimum Sobolev norm (MSN) Chebyshev interpolation method as a numerically sound scheme for computing interpolating polynomials on unstructured grids with guaranteed convergence properties (no Runge phenomenon). For higher rates of convergence we use increasingly ill-conditioned matrices coupled with specialized high relative-accuracy solvers. The resulting algorithm is accurate but $O(n^3)$. We report on efforts to speed it up using FMM techniques.

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MS121

Efficient Preconditioners and Hierarchical Interpolative Decompositions

In this talk, we will discuss our recent progress on developing efficient preconditioners for partial and integral equations based on hierarchical interpolative decompositions.

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MS121

Optimal Complexity Fast Volume Integral Equation Solvers in Electromagnetics

The notion of fast Integral Equation (IE) solvers is built on the compressibility of the low-rank off-diagonal dense blocks. Knowing that minimal rank comes from cubic complexity SVD, in this talk, I will present how linear complexity iterative (for arbitrary frequency) and direct (low-frequency) VIE solvers are developed using our novel linear complexity SVD rank-compression algorithms for H2(Hierarchical) matrices in electromagnetics. First ever O(NlogN) high frequency direct IE solver will also be presented.

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MS122

A Conservative Semi-Lagrangian HWENO Method for the Vlasov Equation

In this talk, we will present a high order conservative semi-Lagrangian (SL) Hermite weighted essentially non-oscillatory (HWENO) method for the Vlasov equation based on dimensional splitting [Cheng and Knorr, Journal of Computational Physics, 22(1976)]. The major advantage of HWENO reconstruction, compared with the original WENO reconstruction, is compact. For the split one-dimensional equation, to ensure local mass conservation, we propose a high order SL HWENO scheme in a conservative flux-difference form, following the work in [J.-M. Qiu and A. Christlieb, Journal of Computational Physics, v229(2010)]. Besides performing dimensional splitting for the original 2D problem, we design a proper splitting for equations of derivatives to ensure local mass conservation of the proposed HWENO scheme. The proposed fifth order SL HWENO scheme with the Eulerian CFL condition has been tested to work well in capturing filamentation structures without introducing oscillations. We introduce WENO limiters to control oscillations when the time stepping size is larger than the Eulerian CFL restriction. We perform classical numerical tests on rigid body rotation problem, and demonstrate the performance of our scheme via the Landau damping and two-stream instabilities when solving the Vlasov-Poisson system.

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MS122

Maximum-Principle-Satisfying Third Order Direct Discontinuous Galerkin Methods for Time Dependent Convection Diffusion Equations on Unstructured Triangular Mesh

In this talk, the third order maximum-principle-satisfying (MPS) Direct discontinuous Galerkin methods (DDG) for convection diffusion equations on unstructured triangular mesh are presented. The key contribution of DDG is the introduction of numerical flux to approximate the solution derivative at the discontinuous element boundaries. We carefully calculate the normal derivative numerical flux across the element edges and prove that with proper choice of parameters in the numerical flux, the piecewise quadratic polynomial solution satisfies strict maximum principle and maintains the third order accuracy at the same time. The implementation is very efficient, with a simple MPS limiter applied after each time stepping. There are potential applications in physical models which require the solutions satisfying maximum principle or preserving positivity during time evolution. Numerical examples including incompressible flows will be presented as well in the talk.

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MS122

An Asymptotic Preserving Maxwell Solver Resulting in the Darwin Limit of Electrodynamics

In plasma simulations, where the speed of light divided by a characteristic length is at a much higher frequency than other relevant parameters in the underlying system, such as the plasma frequency, implicit methods begin to play an important role in generating efficient solutions in these multi-scale problems. Under conditions of scale separation, one can rescale Maxwell's equations in such a way as to give a magneto static limit known as the Darwin approximation of electromagnetics. In this talk, we present a new approach to solve Maxwell's equations based on a Method of Lines Transpose formulation, combined with a fast summation method with computational complexity O(NlogN), where N is the number of grid points. Under appropriate scaling, we show that the proposed schemes result in asymptotic preserving methods that can recover the Darwin limit of electrodynamics.

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MS122

A Conservative Sweeping Method for Enforcing Maximum Principle

In this talk, we will talk about a conservative bound-preserving sweeping procedure. The main advantage is the simplicity of implementation while maintaining the high order of accuracy. Numerical examples are provided to show the performance and efficiency of the procedure.

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MS123

Collaborative Data Analytics with DataHub

Increasingly, scientific computing relies on groups of researchers to collaboratively clean, curate, and analyze datasets. This is often an ad-hoc process that results in many copies of the dataset files with file naming and out of process communication to coordinate and track modifications. Such approaches create significant redundancy and limit the ability to incorporate concurrent work on the same dataset. To address these issues we propose a collaborative analytic data platform with dataset versioning, DataHub.

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MS123

Big Data in High Throughput Screening

Our group developed specialized robotic microscopes that generate high throughput longitudinal single cell imaging data around the clock for phenotypic genetic and small molecule screening. Collectively, the systems generate more than 10Tb of data a day. In this talk, we will discuss the challenges these systems create for automated data analysis and storage and the implementation of machine learning and other tools for feature extraction and data mining.

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MS123

Linking and Mining Electronic Health Records and Claims Data to Understand Patterns of Care

Electronic Health Records and Claims data (billing data from government and commercial health plans) together provide the ability to understand the responses over time to a treatment for a large number of patients. Key challenges in doing this are de-duplication of patients across multiple health care systems and matching patients against claims data, ideally in a privacy-preserving manner. This talk will describe our experiences in data linking and mining to understand patterns of care.

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MS123

Secondary Use of an Eighty-Billion-Row Clinical Data Warehouse

MAVERIC is a Veterans Health Administration center that runs clinical studies and innovates in clinical practice. Much of our work based on medical record data uses the VA Corporate Data Warehouse, which features twenty million unique patient records, 1000 data tables, and 20,000 columns, aggregated from 130 sites with minimal central integration/harmonization. We will discuss approaches to challenges such as data cleaning or deduplication, scaling our processes, and managing reidentification risk.

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MS124

Time-Integrating PDEs Faster by Tessellating Space-Time Better

Future engineers will design economic and capable aerospace vehicles and engines using high fidelity simulations. To enable this future, such simulations must run significantly faster than today. What prevents simulations from running faster is no longer just the amount of computation power. Communication latency between processors is becoming a main barrier for simulations based on partial differential equations. In this talk, we will illustrate how we can decompose space and time in non-conventional fashions, to effectively break the latency barrier, while using many existing numerical schemes. We will also discuss how to use this technology to accelerate existing, validated simulation software by refactoring the source code.

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MS124

A Parallel Space-Time Solver for the Time-Periodic Navier-Stokes Problems

We are investigating methods for solving time-periodic Navier–Stokes problems, i.e. flows which are excited by a periodic forcing. After multiple periods of the forcing cycle the resulting flow field can converge toward a time-periodic steady state. This steady-state solution can be approximated by a truncated Fourier series in the time domain, such that every Fourier coefficient is a function in space. We obtain a big nonlinear system of equations, which is solved in parallel with respect to space and time.

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MS124

Dirichlet-Neumann Neumann-Neumann Waveform Relaxation

Recently several waveform relaxation algorithms have been proposed, where the standard Dirichlet or Robin coupling conditions are replaced by transmission conditions that are implemented in stages, for example the Dirichlet–Neumann coupling conditions. These new transmission conditions promise better rates of convergence at the expense, as it turns out, of parallel efficiency. This talk focuses on a practical implementation of these new waveform relaxation algorithms, as well as an analysis of the communication cost and efficiency overhead of these algorithms.

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MS125

The Bounds on the Risk Premium of Markovian Pricing Kernels and the Recovery with Transient Processes

Many authors have suggested the extension of Ross model to continuous time setting under specific circumstance, which, in particular, guarantee the uniqueness of the measure. Especially, the recovery is achieved under some classes of pricing kernel with conditioned stochastic processes. In this talk, we will discuss the possibility of recovery when the process is transient by analyzing the corresponding second order differential equations and, furthermore, the bounds of the risk premium under the relaxed constraint of the process.

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MS125

Calculating the Greeks with the H-Transform

In this talk, a sensitivity analysis of long-term cash flows with respect to perturbations in the underlying process is presented. For this purpose, we employ the h-transform through which a pricing operator is transformed into what is easier to address. The method of Fournie will be combined with the martingale extraction. We prove that the sensitivity of long-term cash flows can be represented in a simple form.

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MS125

Optimal Retirement Plan on a Finite Horizon

This paper considers a utility of spending scaled by the past peak spending, and solves an optimal spending-investment problem in a finite horizon. A closed form solution suggests that the spending rate is constant and equals the historical peak for relatively large values of wealth/peak consumption, decreases when the ratio is relatively small, and in particular, increases when the ratio reaches an upper bound.

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MS125

Endogenous Current Coupons

We consider the problem of identifying current coupons for Agency backed To-be-Announced pools of residential mortgages. In a doubly stochastic reduced form model which allows for prepayment intensities to depend upon both current and origination mortgage rates, as well as underlying investment factors, we identify the current coupon with solutions to a non-linear fixed point problem. Using Schaefer's theorem we prove existence of current coupons. We also provide an explicit approximation to the fixed point.

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MS126

Polynomial Continuation Techniques for Equations Arising from Nonlinear Optimization

Given a finite collection of subspaces $\mathcal{C}$ of a finite-dimensional vector space $\mathcal{V}$ how do we represent $\mathcal{C}$ by a one-dimensional vector space ℓ? A common strategy is to formulate a nonlinear optimization problem. Motivated by an image classification problem, we consider the case when the objective function is a sum of cosines of principal angles between $\mathcal{C}$ and ℓ. This problem is equivalent to the *multivariate eigenvalue problem*. We will share polynomial continuation methods that solve this highly structured problem.

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MS126

Computing Small Certificates of Inconsistency of Quadratic Fewnomial Systems

We study systems of n multivariate quadratic equations that only use a small subset M of monomials. We focus on generic systems that do not admit any solution at all. We show that if the cardinal of M is less than $n - 1/2 + (1/4 + 2N)^(1/2)$ (where N is the matching number of a graph associated with M) then there exists a certificate of inconsistency of linear size, which can be computed in polynomial-time. We provide experimental results for systems with more than 30000 variables and equations.

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MS126

Singular Vectors of Tensors

The singular valued decomposition (SVD) of a matrix is very useful in a wide range of applications. Recently there has been significant interest in extending key properties of this decomposition to the higher-dimensional tensor setting. In this talk we define a singular vector of a tensor. We describe the geometry of tuples in projective space that can occur as the singular vectors of a tensor.

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MS126

Learning Directed Acyclic Graphs Based on Spars-

est Permutations

We consider the problem of learning a Bayesian network or directed acyclic graph (DAG) model from observational data. We propose the sparsest permutation algorithm, a nonparametric approach based on finding the ordering of the variables that yields the sparsest DAG. We prove consistency of this method under strictly weaker conditions than usually required. We discuss how to find the sparsest ordering by introducing the DAG associahedron and a simplex-type algorithm on this convex polytope.

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MS127

Locally Optimized Covariance Kriging for Engineering Design Exploration

Kriging is commonly used to alleviate the high computational cost associated with engineering design explorations, e.g. uncertainty quantification and multidisciplinary design optimization. In this talk, the locally optimized covariance Kriging (LOC-Kriging) method is introduced to capture the non-stationarity of the underlying function. In LOC-Kriging, the non-stationarity is identified with a statistical test process and approximated by aggregating a finite number of locally optimized stationary covariance structures within the design domain of interest.

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MS127

Gradient-Enhanced Kriging Model for Large Data Set: A New Formulation

Gradient-enhanced surrogate modeling has received much attention in the research area of aerodynamics, due to the availability of inexpensive gradient computation method such as adjoint method. Theoretically, the so-called gradient-enhanced kriging (GEK) model can greatly improve the efficiency of building a sufficient accurate surrogate model in high dimensions using the cheap gradient computed by adjoint method. However, in reality, the building of GEK model is suffering from the problem associated with inversing large correlation matrix, which has greatly limited the application of GEK model for aerodynamic problems. This paper proposes a new formulation of GEK model to work out this problem. The main idea is to build a series of GEK sub-models with much smaller correlation matrix, then sum them up with appropriate weight coefficients and the final surrogate model is obtained. We make a self-contained derivation about the formulation of the new GEK model. The new GEK model is verified by analytical problems as well as the building of a surrogate model for drag coefficient of an RAE2822 airfoil, with adjoint method computing the gradients. It is shown that the accuracy of GEK model is only slightly decreased, while significantly improving the efficiency of building the model. The new GEK model is applied to wing shape inverse design based on target pressure distribution and has been proved to be efficient in the optimization within high dimensional design space.

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MS128

Numerical Methods for Exploring Parameter Spaces

Problems from a variety of application areas can be represented by parameterized polynomial systems. Some of these problems then translate into the problem of finding points or regions of interest within the parameter space. Numerical methods rooted in homotopy continuation provide a means for finding such points and regions. This talk will focus on recent approaches of this sort, motivated by and applicable to various applications in systems biology.

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MS128

A Case Study in Algebraic Systems Biology

Steady state analysis of dynamical systems for biological networks give rise to algebraic varieties in high-dimensional spaces whose study is of interest in their own right. For example, the variety corresponding to the shuttle model of the Wnt signaling pathway is described by a polynomial system in 19 unknowns and 36 parameters. Using the Wnt signaling pathway shuttle model as an example, we will translate biological questions into algebraic ones and illustrate the different ways that computational algebraic geometry and combinatorics can be used to better understand a given model. This is joint work with Heather Harrington, Zvi Rosen, and Bernd Sturmfels.

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MS128

Algebraic Complexity in Gene Regulation

The regulatory behaviors of genes can be expressed as rational functions of transcription factor concentrations. We will describe several conjectures about such functions, which are suggested by numerical calculations, and show that an algebraic complexity barrier arises when energy is consumed for regulatory purposes, as is typical in eukaryotes, which must be overcome if we are to understand how genes work.

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MS128

Which Biochemical Reaction Networks Are Multistationary?

Many dynamical systems arising in systems biology are multistationary, and yet the following question is open:

when taken with mass-action kinetics, which reaction networks have the capacity for two or more steady states? No complete answer is known. In this talk, we answer this question for the smallest networks. Our results highlight the role played by the Newton polytope of a network (the convex hull of the reactant vectors).

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MS129

Computational Methods for Extremal Steklov Problems

We develop a computational method for extremal Steklov eigenvalue problems and apply it to study the problem of maximizing the p-th Steklov eigenvalue as a function of the domain with a volume constraint. In contrast to the optimal domains for several other extremal Dirichlet- and Neumann-Laplacian eigenvalue problems, computational results suggest that the domain maximizing the p-th Steklov eigenvalue is unique (up to dilations and rigid transformations), has p-fold symmetry, and an axis of symmetry.

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MS129

A High-Order Perturbation of Surfaces/Asymptotic Waveform Evaluation (HOPS/AWE) Method for Two-Dimensional Grating Scattering Problems

The scattering of electromagnetic waves by periodic gratings is important in applications. High-Order Perturbation of Surfaces (HOPS) methods were devised by Milder and Bruno & Reitich for the rapid and robust simulation of these interactions. With a single simulation, for fixed illumination frequency, these methods produce returns for an arbitrary selection of grating heights. We describe a novel HOPS/Asymptotic Waveform Evaluation algorithm which, with a single computation, generate simulations for arbitrary depth and frequency granularity.

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MS129

Domain Decomposition Methods for the Solution of Multiple Scattering Problems

We present an efficient Domain Decomposition Method for the solution of time-harmonic scattering by multiple obstacles. The main idea in the algorithm is to algebraically merge Robin to Robin maps for adjacent subdomains in a hierarchical manner. The Robin to Robin maps are computed efficiently using well-posed boundary integral equations.

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MS129

Nonlinear Photoacoustic Tomography with Two-Photon Absorption

The objective of photoacoustic tomography is to reconstruct optical properties of heterogeneous media from measured acoustic signals generated from the photoacoustic effect. We present in this talk some mathematical and numerical studies on nonlinear photoacoustic tomography based on the two-photon absorption principle. We will show some uniqueness and stability results on the inverse problem, as well as some numerical simulations based on synthetic data.

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MS130

Using Case Studies to Integrate Modeling into Biocalculus Classes

There is a growing demand for mathematics and statistics courses tailored to life-science students. I will discuss how real-world case studies can be used to provide a richer integration of biology with mathematics. An example focusing on vaccination and pathogen evolution will be presented that illustrates how one can motivate the development of several mathematical ideas from calculus and tie them together through modeling.

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MS130

Can You Build a Taj Mahal Out of Lego Blocks? Teaching Systems and Simulation Modeling to Graduate Students in Ecology

Computational models are important for addressing problems in applied ecology, such as species conservation, ecosystem restoration, and sustainable harvesting. How do should we train ecology students to build and apply simulation models of appropriate complexity, particularly those students with limited quantitative training? Here we discuss the bare essentials of the quantitative concepts needed by these students, and the type of software they will ultimately need to be effective modelers in their applied ecologist careers.

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MS130

Some Lessons from 40 Years of Quantitative Education for Biologists

Many efforts over several decades have attempted to enhance quantitative components of the biology curriculum. A "curriculum" is not a list of courses but rather a plan for interactions between students, faculty, and materials to meet a collection of learning objectives. I will discuss methods to develop a feasible undergraduate curriculum that accounts for the interdisciplinary nature of modern life sciences and the diversity of quantitative skills and conceptual knowledge required.

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MS130

Preparing for a Quantitative Job in the BioPharma Industry

A new employee in industry is often hired to immediately contribute to project goals. For example, a company developing stroke-prevention treatments may hire a mathematician with experience creating ODE cardiovascular models to simulate different scenarios. This requires expertise in: mathematical systems modeling; computer programming; and anatomy, tissue function, and disease states. I will discuss the training expected for certain quantitative jobs in the biopharma industry, and some additional advice on finding such jobs.

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MS131

The Effective Dispersion Relation for the Nonlinear Schrodinger Equation

The linear part of the Nonlinear Schrödinger Equation (NLS) ($iq_t = q_{xx}$) has dispersion relation $\omega = k^2$. We don't necessarily expect solutions to the NLS to behave nicely or have any kind of effective dispersion relation. However, I have seen that solutions to the NLS are actually weakly coupled and are often nearly sinusoidal in time with a dominant frequency, often behaving similarly to modulated plane waves. I will show a number of plots regarding this.

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MS131

The Role of Geometry in Controlling Asymmetries in Passive Scalar Transport

We explore the role different geometries (amongst rectangular and elliptical domains of arbitrary aspect ratios) play in controlling emerging up-stream/downstream asymmetries in the cross-sectionally averaged distribution of diffusing passive scalars advected by laminar, pressure driven shear flows. We show using a combination of rigorous analysis, asymptotic expansions, and Monte-Carlo simulations, that on short time scales relative to the shortest diffusion times, elliptical domains preserve initial uptream/downstream symmetric distributions, while rectangular ducts break this symmetry. Skinny ducts produce distributions with negative skewness, while fat ducts produce positive skewness for symmetric initial data which is uniformly distributed in the cross-section. There is a special aspect ratio of approximately 2-1 ratio for which symmetry is preserved. In turn, long-time (relative to the longest diffusion timescale) exact analysis shows that all geometries generically break symmetry before ultimately symmetrizing in infinite time.

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MS131

Causes of Metastability and Their Effects on Transition Times

Many experimental systems can spend extended periods of time relative to their natural time scale in localized regions of phase space, transiting infrequently between them. This display of metastability can arise in stochastically driven systems due to the presence of large energy barriers, or in deterministic systems due to the presence of narrow passages in phase space. To investigate metastability in these different cases, we take the Langevin equation and determine the effects of small damping, small noise, and dimensionality on the dynamics and mean transition time.

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MS131

Waveaction Spectra and Effective Dispersion of Fully Nonlinear Mmt Model

We investigate a version of the Majda-McLaughlin-Tabak model of dispersive wave turbulence where the linear term in the time derivative is removed. We consider driven-damped and undriven, undamped cases of the model. Our theoretical predictions for the waveaction spectrum, which are made using statistical mechanical methods as well as arguments reminiscent of Kolmogorov's theory of turbulence, are found to agree with time dynamics simulations.

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MS132

Electrohydrodynamics of a Planar Lipid Bilayer Membrane

Lipid bilayer membrane is a key cellular component. Made of two layers of amphiphilic lipid molecules, the bilayer lipid membrane has an elastic bending stiffness and a capacitance. Often modeled as a capacitive elastic sheet due to the small thickness of the bilayer (5 nm), the electrohydrodynamics (EHD) of a lipid bilayer membrane under an electric field is essential to understand electrodeformation and electroporation of vesicles (self-enclosing lipid membranes) and cells. To understand the lipid membrane EHD we first utilize the leaky dielectric framework to describe both the linear and weakly nonlinear dynamics of a lipid membrane in fluids mostly charge neutral except near the interface. We then show how relaxation of this assumption may lead to different membrane EHD.

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MS132

Vesicles in Electric and Magnetic Fields

Vesicles undergo interesting dynamics when exposed to electric or magnetic fields. Electric fields induce large deformation in the vesicle membrane and alignment of vesicles in magnetic fields have also been demonstrated. Here, a recent numerical model of vesicles is presented that allows for the magneto-electro-hydrodynamics of vesicles. The model, sample results, and possibilities for future work will be outlined.

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MS132

Numerical modelingn of the Electrohydrodynamic of a Viscous droplet

We present a novel numerical approach for the simulation of viscous drop placed in an electric field in two and three spatial dimensions. Our method is constructed as a stable projection method on Quad/Octree grids. Using a modified pressure correction we were able to alleviate the standard time step restriction incurred by capillary forces. In weak electric fields, our results match remarkably well with the predictions from the Taylor-Melcher leaky dielectric model. In strong electric fields the so-called Quincke rotation is correctly reproduced.

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MS132

Computational Modeling of Osmotic Water Flow with Moving Interfaces

We develop a computational framework to simulate ionic electrodiffusion and osmotic water flow in cellular systems. In the biological model system we used, cell membranes, which are permeable to both water and ionic flows, divide the domain into intracellular and extracellular regions. The cell membranes move with the flow it is embedded in, while its elastic force and osmotic forces due to ions will in turn affect fluid properties. The model system then include fluid-structure interactions and ionic electrodiffusion on domain with moving (internal) interfaces. The computation of advection-diffusion in a 2d rectangle domain with moving boundaries is carried out by using a embedded Cartesian grid method over the entire rectangle domain, which represents the intra- and extracellular regions, while the fluid-structure interactions is handled by the Immersed Boundary Method. We will describe our numerical scheme of solving this PDE system and illustrate the results with some simple applications as the proof of principles.

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MS133

High-Order Algorithms for Caputo Derivatives and Caputo-Type Partial Differential Equations

Abstract Not Available at Time of Publication

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MS133

Backward Fractional Diffusion Equation

The fractional diffusion equation replaces the second spatial derivative in the traditional diffusion equation with a fractional derivative of order between 1 and 2. It governs a stable Lévy process (Lévy flight), a natural analogue of Brownian motion. Particle density spreads faster than the Brownian model, with a heavy leading tail in the flow direction. The model has found practical applications to turbulence, hydrology, biology, medical imaging, and finance. This talk presents the corresponding backward equation, which can be used to identify the initial particle location and release time. The backward method is developed from the theory of inverse problems, and then explained from a stochastic point of view. This backward equation differs significantly from the traditional backward diffusion equation, because the fractional derivative is not self-adjoint. Hence the likelihood function for backward locations is highly skewed. The method will be illustrated with an application to groundwater hydrology.

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MS133

Fast Numerical Methods for Space-Time Fractional Pdes

Abstract Not Available at Time of Publication

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MS133

Petrov-Galerkin Spectral Methods for Distributed-Order Fractional PDEs

Abstract Not Available at Time of Publication

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MS134

A Peridynamic Model for Hydraulic Fracture

We present a coupled nonlocal model based on peridynamic theory for the poromechanical deformation and failure of rocks targeting applications of hydraulic fracture. The model is capable of reproducing known analytic solutions to simple fracture geometries as the characteristic nonlocal length-scale vanishes; however, the nonlocal nature of the formulation is particularly useful in regularizing (i.e., removing mesh dependence) cases of complex fracture propagation and coalescence of propagating hydraulic fractures with natural fractures. This presentation will shows the model equations along with validation results for a series of test problems. Additionally, we show regularized large-scale simulations that exhibit sufficient complexity to demonstrate the utility of the model. This complexity includes the effects of heterogeneities in elastic, fracture, and fluid transport properties, as well as the effects of complex natural fracture networks on hydraulic fracture propagation.

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MS134

An Implicit Corrected SPH Formulation for Fluid Flow in Anisotropic Porous Media

The reservoir simulation of the complex reservoirs with anisotropic permeability is a major challenge. The smoothed particle hydrodynamics (SPH) method has proven useful for modeling different physical phenomena. This paper presents the meshless approximation of second order elliptic operator containing a tensor coefficient. The proposed meshless description is tested by solving steady-state and transient problems of fluid flow in anisotropic porous media using the Backward Euler method with a GMRES solver.

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MS134

Construction of Optimal Multi Scale Basis Functions for Partition of Unity Methods

The approximation power of a generalized finite element method or partition of unity method essentially stems from the use of problem-dependent enrichment functions. In the context of problems with micro-structure such enrichment functions must be employed on the whole domain and capture the effects of the micro-structure. We present a general framework for the construction of such enrichments and compare the performance of different multi scale approaches in this context.

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MS134

A Partition of Unity Method for the Propagation of Hydraulic Fractures With/Without Lag

The simulation of hydraulic fractures implies challenges such as solving a non-linear system of equations in an efficient way or high pressure gradients for small or vanishing fluid lag. We present an implementation based on a flat-top PUM where enrichments can be used to gain good approximations with even only few DOF while retaining stability. We give results in 2D and 3D. Solving of the non-linear systems of equations involves an iterative multilevel solver.

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MS135

Dynamics of Water Use

Social, environmental, and economic factors all influence the sustainability and use of common pool resources, such as water. When modelling such systems, these complexities can make it challenging to use traditional mathematical models defined by ordinary differential equations with particular functional forms. I review generalized modelling as a technique to answer questions about the stability and optimal allocation of water as a resource.

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MS135

Inferring Offline Social Networks from Online Data

We explore how data from the online social media website Meetup can be used to infer the structure of offline social networks. Meetup users form online groups and attend offline events, allowing for correlations to be found between online and offline activity. We investigate how social activity of subnetworks varies on the choice of city and the interests of users. Applications to modeling the spread of infectious diseases and the diffusion of information will be discussed.

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MS135

Stochastically Driven Plant Biomass and Soil Moisture Dynamics in Water-Limited Ecoystems: Analytical Results

When the joint system of soil moisture and plant biomass (which are coupled via transpiration) is driven by a random rainfall process, distributions of both quantities are induced. We derive a new analytical result for these distributions, and show how their behavior is influenced by the key hydrologic and physiological parameters. Specific attention is given to how this probabilistic description helps to characterize growth feedbacks, which can manifest as, e.g., bimodal biomass distributions.

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MS135

Velocity Estimation Using Multi-Level Monte Carlo Bayesian Inversion

Seismic inversion attempts to use data collected on the Earth's surface to infer information about the subsurface. A Bayesian approach to subsurface velocity field inversion can reveal information about lithology and associated uncertainty. However, it is computationally expensive. We propose a multilevel Markov chain Monte Carlo method to reduce computational costs while retaining necessary information for uncertainty quantification. An upscaled acoustic wave equation solver is used to quickly and cheaply filter unacceptable velocity field proposals.

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MS136

Parallelization of the Rational Arnoldi Method

The rational Arnoldi algorithm is a popular method in scientific computing used to construct an orthonormal basis of a rational Krylov space. Each basis vector is a rational matrix function times the starting vector. Rational functions possess a partial fraction expansion which often allows to compute several basis vectors simultaneously. However, this parallelism may cause instability due to the orthogonalization of ill-conditioned bases. We present and

compare continuation strategies to minimize these effects.

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MS136

Block Preconditioned Thick-Restart Lanczos Method with Subspace Optimization for Symmetric Eigenvalue Problems

We propose a new near-optimal eigenmethod, TRLAN+K, that combines the efficiency of the Lanczos algorithm and the power of the subspace optimization techniques. The proposed method can also take advantage of a preconditioner. We use an inverse-free type preconditioned Krylov subspace scheme. Finally, a block preconditioned TRLAN+K is presented. Numerical experiments show that the proposed method can achieve almost optimal convergence and converge up to ten times faster than TRLAN under limited memory.

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MS136

Spectrum Slicing by Polynomial and Rational Function Filtering

Two filtering techniques are presented for solving large eigenvalue problems by spectrum slicing. In the first approach, the filter is constructed as the least-squares approximation to an appropriately centered Dirac distribution. In the second approach, a least-squares rational filter is designed for matrices whose spectrum is contained in a large interval and generalized eigenvalue problems.

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MS136

A Contour-Integral Based Structured Eigensolver for Non-Hermitian Matrices

We propose a fast (nearly $(O)(n^2)$ cost) contour-integral based structured eigensolver for a class of structured non-Hermitian matrices, it is based on hierarchically semiseparable (HSS) representation and projected subspace iteration. We discuss the design of a filter function and compare different quadratures have been used before. Structures can be utilized to largely accelerate various processes in the solver. This is joint work with Jianlin Xia and Raymond Chan.

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MS137

Control for Systems With Uncertain Parameters through Reduced Order Models

We present work on data-driven surrogate models for online control of complex systems modeled through parameter dependent PDEs. Such systems present big challenges for model-based control and observer design, since system dynamics often change significantly with the underlying model parameters (e.g., viscosity in fluids). A data-driven framework allows us to update reduced order models with real data to account for parametric changes online, and subsequently use the model for the control task at hand.

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MS137

A Certified Reduced Basis Approach to PDE-constrained Parameter Optimization

PDE-constrained parameter optimization problems often require a prohibitively large number of computationally expensive PDE solves. It is therefore advantageous to replace expensive PDE solvers with lower-dimension surrogate models. In this talk, we use the reduced basis (RB) method in conjunction with a trust region optimization framework. New RB error bounds are used to ensure convergence of the proposed approach. We consider problems governed by elliptic PDEs and present numerical results for a thermal fin model.

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MS137

A Certified Reduced Basis Method for Variational Inequalities and Optimal Control Problems

First, we present a minimum residual, slack-variable RB approach for variational inequalities. The proposed method provides error bounds which are significantly sharper than existing bounds; and it enables a full offline-online computational decomposition. Second, we discuss the use of ROMs for PDE-constrained optimal control problems. We develop rigorous and efficiently computable error bounds for both the distributed optimal control and the optimal cost functional. Numerical results compare the performance of the proposed and existing approaches.

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MS137

A Globally Convergent, Inexact Trust-Region Method for Optimization Under Uncertainty using Sparse Grids and Model Reduction

This work introduces a framework for accelerating optimization problems governed by partial differential equations with random coefficients by leveraging adaptive sparse grids and model reduction. Adaptive sparse grids perform efficient integration approximation in a high-dimensional stochastic space and reduced-order models reduce the cost of objective-function and gradient queries by decreasing the complexity of primal and adjoint PDE solves. A globally-convergent trust-region framework accounts for inexactness in the objective and gradient.

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MS138

A Bayesian Approach to Understanding the Effects of a Fatal Virus Disease on Gypsy Moth Populations

Gypsy moth populations periodically rise to high densities, leading to widespread defoliation, before being decimated by a viral pathogen. To understand the role of small-scale transmission in virus epidemics, we used single-branch experiments to construct informative priors for the parameters of stochastic epidemic models. We then used WAIC to show that models with informative priors better explain epidemic data than models with uninformative priors. Small scale transmission thus plays a key role at larger scales.

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MS138

Cannibalism and Disease Transmission: How Risky is it to Eat your Own?

Cannibalism, while prevalent in the biological world, is often viewed as detrimental to the health of an individual. By cannibalizing weak or sick individuals, the chance of coming into contact with a pathogen and subsequently becoming infected with that pathogen increases. Using a series of experiments and mechanistic models at a variety of scales, we demonstrate that cannibalism potentially slows disease spread during an outbreak and, therefore, may not be as deleterious as once thought. It may even be advantageous.

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MS138

Managing Multiple Sources of Uncertainty: Optimal Outbreak Response for Foot-and-Mouth Disease

Decision-makers face a trade-off between learning through continued observation of an outbreak and the opportunity cost of inaction. We develop an adaptive control policy that responds to changing information about competing dynamical models (posterior distributions) and changing epizootiological states (size and spatial extent of an outbreak). We achieve the former through a sequential analysis of real-time outbreak surveillance and the latter using reinforcement learning to solve for an optimal state-dependent control policy for a spatially explicit livestock outbreak.

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MS138

Effects of Biodiversity on Disease Outbreaks: The Importance of Decreasing Variability in Transmission

Empirical and theoretical research has demonstrated that increasing host biodiversity decreases disease transmission, known as the dilution effect. This effect, however, only considers changes in the mean transmission rate, not the variability associated with transmission. By combining statistical and mathematical models with data, we examine how increased biodiversity in a tri-trophic system can lead to more consistent outcomes. Thus the dilution effect may be driven by changes in the mean and the variability of transmission.

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MS139

Computational Methods for Local and Non-Local Hydrodynamic Models for Phase Transitions

This talk will consider a class of hydrodynamic models for solid liquid phase transitions that arise from Kinetic Density Functional Theory of freezing. These models take the form of compressible Stokes or Navier Stokes equations driven by gradients in chemical potential. These chemical potential may be local or non-local functionals of the density field. The talk will outline the development of implicit unconditionally energy stable finite difference methods within the framework of convex splitting schemes. Challenges in preserving positivity of the density field will addressed. Some applications illustrating the ability of the methods to capture the effect of flow on solid-liquid phase transitions will also be discussed.

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MS139

A Particle-Cluster Cartesian Treecode for Multipolar Electrostatic Interactions in Molecular Simulations

Multipolar electrostatic interactions have been shown to provide better accuracy than fixed point charged models for several problems in computational chemistry. However, even simulations employing lower order multipoles (dipoles or quadrupoles) are significantly more computationally intensive than fixed point charge models. We present an $O(N\log N)$ Cartesian treecode algorithm developed to speed up N-body particle-particle multipolar electrostatic interactions in order to relieve the computational bottleneck.

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MS139

Developing a Lagrangian Particle Method for Geophysical Applications

The development of a Lagrangian Particle Method (LPM) for geophysical applications is discussed for various problems including tracer transport, vorticity dynamics in rotating flow, and shallow water gravity waves. The LPM is based on Vortex Methods, numerical techniques developed for incompressible flow that rely on the point vortex approximation. A Poisson equation relates the stream function to vorticity and is solved using a Green's function integral. Velocity is computed from the related Biot-Savart integral and a quadrature scheme on a finite set of moving particles (point vortices). A new remapping procedure is applied at regular time intervals to maintain spatial accuracy and minimize error due to particle distortion. Particles are inserted and removed adaptively to maintain resolution of the flow as small-scale features develop. The challenge of extending these techniques to flows with nonzero velocity divergence using Particle Strength Exchange (PSE) is discussed. Examples and solutions are presented for planar and spherical geometries and include transport in deformational flow, Rossby-Haurwitz waves, Gaussian vortices, and the interaction of gravity waves with topography.

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MS139

Pros and Cons of Cartesian Treecode and Fast Multipole Method

Fast Multipole Method (FMM) and Treecode are popular tree-based algorithms with rigorous error estimate and wide applications in computing N-body particle interactions. FMM takes both near-field and far-field expansions, resulting in the revolutionary $O(N)$ computations. Treecode takes only the far field expansion, receiving less efficient $O(N(\log N))$ computations in trade of saved memory and improved parallelization efficiency. This project compares both methods under the Cartesian expansion in terms of efficiency, memory use, and parallel performance.

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MS140

Vortices in P-Wave Superconductivity

We study vortices in p-wave superconductors in a Ginzburg-Landau setting. The state of the superconductor is described by a pair of complex wave functions, and the p-wave symmetric energy functional couples these in both the kinetic (gradient) and potential energy terms, giving rise to systems of partial differential equations which are nonlinear and coupled in their second derivative terms. We prove the existence of energy minimizing solutions in bounded domains $\Omega \subset \mathbb{R}^2$, and consider the existence and qualitative properties (such as the asymptotic behavior) of equivariant solutions defined in all of $\mathbb{R}^2$. The coupling of the equations at highest order changes the nature of the solutions, and many of the usual properties of classical Ginzburg-Landau vortices either do not hold for the p-wave solutions or are not immediately evident.

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MS140

Approximate Global Minimizers for Pairwise Interaction Problems

In this talk I will examine a general class of model functionals: those arising in non-local pairwise interaction problems. I will present a new approach for computing approximate global minimizers based on a convex relaxation of the underlying energy landscape, along with a recovery technique. The approach is sometimes exact, and also provides a numerical recovery guarantee for the approximate minimizer that is often within a few percent of the global minimum. The approach sometimes predicts exact lattice minimizers, and generates a dual decomposition for the energy landscape that leads to the emergence of new preferred low energy length scales.

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MS140

Periodic Orbits to Gross Pitaevskii in the Disc with vortices following Point Vortex Flow

In this talk we describe two approaches to constructing time periodic solutions to the Gross-Pitaevskii (GP) equations on the unit disc- the first based on constrained minimization and the second based on topological linking. Our motivation in doing this is to build a connection between periodic orbits to the Point vortex flow that's valid for all time– indeed, the problem considered serves as a first example to understand and relate long time behavior of Gross-Pitaevskii to the Point Vortex Flow. A crucial advantage of the linking approach is that we can construct periodic solutions to GP containing vortices of degrees ± 1, that persist for all time without succumbing to vortex annihilation.

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MS141

Optimizing the Kelvin Force in a Moving Target Subdomain

In order to approximate the Kelvin (magnetic) force, we propose a minimization problem, with a tracking type cost functional, in a moving subdomain. We use the so-called dipole approximation to realize the magnetic field. Here, the location and the direction of the magnetic source are assumed to be fixed. The magnetic field intensity, with limiting pointwise constraints, acts as the optimization variable. We address two specific problems: the first one corresponds to a fixed final time whereas the second one deals with an unknown final time. We prove the existence of solution and thanks to second order sufficient condition, we deduce the local uniqueness to these problems under fairly general assumptions on the data. For the time discretization we use classical backward Euler scheme. For both problems we prove the H^1-weak convergence of this semi-discrete numerical scheme using Γ-convergence. This result does not require second order sufficient condition. In presence of second order sufficient condition, a H^1-strong local convergence result is proved. We report computational results to assess the validity of the numerical methods. As an application, we study the control of magnetic nanoparticles as those used in magnetic drug delivery. The optimized Kelvin force is used to transport the drug to a desired location.

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MS141

Numerical Moments and the Approximation of Fully Nonlinear Second Order Partial Differential Equations

We discuss the numerical moment, a new tool that can be used in designing both methods and/or solvers for directly approximating the viscosity solution of fully nonlinear second order partial differential equations. We provide motivation for the numerical moment as well as corresponding analytic results. We also demonstrate the utility of the numerical moment with numerical tests based on a class of nonstandard LDG and IP-DG finite element approximation methods inspired by the generalized monotone finite difference framework of Feng, Kao, and Lewis.

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MS141

Primal and Mixed Finite Element Methods for Elliptic PDEs in Non-Divergence Form

n this talk, we describe a class of finite element methods for $W^{2,p}$ strong solutions of second-order linear elliptic PDEs in non-divergence form. The main novelty of the method is the inclusion of an interior penalty term, which penalizes the jump of the flux across the interior element edges/faces, to augment a nonsymmetric piecewise defined and PDE-induced bilinear form. Existence, uniqueness and error estimate in a discrete $W^{2,p}$ energy norm are proved for the proposed finite element method. This is achieved by establishing a discrete Calderon-Zygmund-type estimate and mimicking strong solution PDE techniques at the discrete level. We provide numerical experiments which confirm the theory, and we discuss possible extensions to fully nonlinear second order PDEs.

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MS141

A Regularized Approach to Adaptivity for Nonlinear PDE in the Coarse Mesh Domain

I will discuss an adaptive framework to approximate nonlinear elliptic PDE starting from a coarse mesh. The target problem class includes quasi-linear problems with steep internal layers in the solution-dependent diffusion coefficients, for which standard techniques to solve the discrete nonlinear problems can fail. The discrete problem on the initial sequence of meshes may be ill-posed, and partial solves of regularized problems are used to refine the discretization. Auto-adaptively updated regularization based on pseudo-time integration and the control of source functions will be discussed.

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MS142

Reimagining Recommendations: Contextual Embeddings from Online Browsing Data

Since the publication of the word2vec algorithm in 2013 (Mikolov, et al, 2013), semantic learning has seen a surge in research. Recent progress has focused on algorithmic improvements, scaling such algorithms to handle ever larger corpora, as well as learning to incorporate novel classes of corpora. In this talk we highlight advances in this area relying on data sources in the context of online commerce.

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MS142

Mining Large Scale Reviews for Consumer Sentiment

With the increasing popularity of online review sites, developing methods to mine and analyze information contained in the vast amounts of noisy user-generated reviews becomes a necessity. We have developed a method to uncover the various aspects of a product or service reviewed by a user, and the opinions associated with them, in an automated fashion. We use the shallow neural network model Word2Vec to build a vector space representation of a large corpus of user-generated, online restaurant reviews, and harness these distributed representations for aspect-based sentiment analysis. User generated text data is intrinsically noisy, with misspellings, informal language, and digressions. Because of the many variations in spelling and expression, the data is also very sparse. Despite these inherent challenges we are able to represent the reviews by key drivers of consumer sentiment, allowing for highly accurate sentiment prediction using a method that is both scalable and human interpretable.

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MS142

Public Opinion Polling with Twitter

Compared to traditional opinion polling techniques, sentiment analysis on text-based data from social media has many advantages. Solicited public opinion surveys are expensive to conduct, poorly resolved in time, and only reflect a limited number of willing participants. In addition, the topics for which survey data are available is rather limited. In this study, we demonstrate that public opinion polling with Twitter correlates well with traditional measures, and has predictive power for several issues of global importance. We also examine Twitters potential to provide unsolicited public opinion polls for topics seldom surveyed, including ideas, personal feelings and commercial businesses.

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MS142

Leveraging Big Data for Societal Well-Being on a Range of Scales

The Big Data community has benefitted from increasingly available and enriched data sources. Data from Facebook and Twitter provide a real-time stream of human consciousness, while traditional sources for societal stories, such as journalistic news feeds, continue to multiply and encompass a more complete world view. Can these rich data sources be leveraged for meaningful measurements at a variety of scales, including individuals, cities, and international relations? We will first present how to use geotagged Twitter data to understand patterns of human mobility and expressed well-being. Secondly, we will demonstrate how social media can be used to estimate real-time census demographics in cities and states. Finally, we will examine an international events dataset allowing for the exploration of international relationships and the identification of the behavioral patterns of nations.

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MS143

Implicit Strong Stability Preserving Runge–Kutta Methods

In this talk we will present prior results on the limitations of implicit Runge–Kutta methods in terms of the SSP conditions, and present new results on SSP implicit RK methods for linear problems, SSP IMEX methods, and implicit SSP RK methods with down winding.

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MS143

Explicit Strong Stability Preserving Multistage Two-Derivative Time-Stepping Schemes

High order strong stability preserving (SSP) time discretizations are advantageous for use with spatial discretizations with nonlinear stability properties for the solution of hyperbolic PDEs. The search for high order strong stability time-stepping methods with large allowable strong stability time-step has been an active area of research over the last two decades. Recently, multiderivative time-stepping methods have been implemented with hyperbolic PDEs. In this work we describe sufficient conditions for a two-derivative multistage method to be SSP, and find some optimal SSP multistage two-derivative methods. While explicit SSP Runge–Kutta methods exist only up to fourth order, we show that this order barrier is broken for explicit multi-stage two-derivative methods by designing a three stage fifth order SSP method. These methods are tested on simple scalar PDEs to verify the order of convergence, and demonstrate the need for the SSP condition and the sharpness of the SSP time-step in many cases.

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MS143

Making SSP Integrators More Practical

State-of-the-art numerical integrators for differential equations are more than just formulas; they come equipped with a range of modern features that make them more efficient and robust. I will discuss recent efforts aimed at developing such features for well-known strong stability preserving (SSP) methods. These features include embedded error estimators and dense output for SSP Runge-Kutta methods and step size adaptivity for SSP linear multistep methods.

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MS143

Efficient Computation of High Derivatives for Multiderivative Methods

Multistage multiderivative methods define a large class of differential equation solvers that contain Runge-Kutta as well as Taylor methods as special cases. In place of introducing additional stages as a Runge-Kutta method typically would to obtain higher order accuracy, multiderivative methods permit the evaluation of derivatives of the solution in addition to the right hand function. Moreover, these methods introduce greater flexibility to Taylor methods by introducing stages that can reduce the total number of derivatives required to obtain a desired order of accuracy. However, one such drawback to these methods for nonlinear problems is the need to compute higher derivatives of the solution which can become quite cumbersome, especially for large problems. In this work, we advocate for the use of differential transforms as well as symbolic tools to automate the entire process.

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MS144

An Overview of Visual Analytics

Visual analytics is the science of combining interactive visual interfaces and information visualization techniques with automatic algorithms to support analytical reasoning through human-computer interaction. People use visual analytics tools and techniques to synthesize information and derive insight from massive, dynamic, ambiguous, and often conflicting data, and to communicate their findings effectively for decision-making. This talk will provide an overview of this emerging field, and introduce some of the most pressing questions facing VA researchers today.

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MS144

Re-Centering Human Centered Visualization

Data visualization is making strides in delivering new tools to users, but providing more options leads to a paradox of choice. One way to address this problem is to better quantify the role of the human in visualization. Towards this end I'll share recent results ranging from low-level perception in visualization, to higher-level concepts like engagement and aesthetics. Re-centering visualization on the human not only aids design, but also brings new opportunities for next-generation visualization systems.

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MS144

Parameter Manipulation for Visualization

Computational tools for statistics and data visualization often make it difficult to modify parameters in analysis. As a result, many users (particularly novices) use default values. I believe full access to parameter manipulation helps both novice and expert users to understand data. I will highlight current tools offering a version of this functionality, and demo a few experimental interfaces I have worked on to show future possibilities in parameter manipulation.

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MS144

Do You See What I See?: An HCI Perspective on Evaluation in Vis

"Data-driven" is now a common modifier across the world of math, science, and journalism. We use visualization as a channel to translate information into human understanding, but how do we know whether a design is effective in the first place? Who (or what) exactly is it effective for? In this talk, I'll discuss common strategies and pitfalls in verifying the design of visualization. These issues motivate a future of evaluation that paints a richer portrait of human interaction.

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MS145

Linear Compartment Models and the Existence of Identifiable Reparametrizations

For a class of linear compartment models known to be unidentifiable, we study the existence of identifiable scaling reparametrizations. Translating previous results to a new criterion based on the rank of a bi-adjacency matrix, we derive new constructions of graphs with an identifiable scaling reparametrization. Using these constructions, a large subclass of such graphs is obtained. Finally, we present a procedure of subdividing or deleting edges to obtain a graph having an identifiable scaling reparametrization.

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MS145

Studying Continuous Conformational Changes of Proteins Using Cryo-EM

Cryo-electron microscopy (cryo-EM) has recently been very successful at producing high resolution 3D models of proteins. Current image processing algorithms in cryo-EM encounter difficulty when the protein being studied exhibits smooth variations of its shape. We will present an overview of several proposed algorithms to study these shape variations and extract 3D 'movies' from cryo-EM images.

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MS145

Combinatorial Interventions for Control Tasks in Large-Scale Signaling Networks

Cellular functions are governed by complex signaling and regulatory networks. Diseases arise from abnormal behavior in these networks. Thus, the design of targeted therapies aims to identify appropriate interventions in these networks, to repress a pathological behavior while minimizing side effects. In this talk we will introduce some approaches to identify and prioritize optimal combinations of interventions for large-scale signaling networks, based on the analysis of the network's structure, using graph theory and combinatorics tools.

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MS145

What Makes a Neural Code Convex?

Neural codes allow the brain to represent, process, and store information. A code is convex if its codewords correspond to regions in an arrangement of convex open sets; such codes have been observed experimentally in many brain areas. Given a particular neural code, how can we tell if it is convex? Using tools from combinatorics and algebra, we uncover signatures of convexity and bounds on the minimal dimension of the underlying space.

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MS146

Cluster-based Reduced-order Modeling and Control of Nonlinear Dynamics

We present a cluster-based reduced-order modelling (CROM) strategy for flow applications. The strategy processes a time-resolved sequence of flow snapshots. We are able to distill physical mechanisms through a refined analysis of the Markov process, e.g. using finite-time Lyapunov exponent and entropic methods. Results are presented for fluid flow applications including control thereof.

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MS146

Inferring Nonlinear Dynamics on Networks from Data

Sparsity-promoting techniques enable system identification of nonlinear dynamics from measurement data. We combine sparse regression of noisy data with an iteratively selected library of functional forms to identify dynamics on networks. Further, we demonstrate how inputs and control can be utilized to identify important measurements and to help in the design of experiments probing system functionality. The framework is tested on metabolic and regulatory biologucal networks.

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MS146

On Nonlinear System Identification for Complex Systems Including Infectious Diseases

Equation-free methods such as Dynamic Mode Decomposition, and it's important connections to Koopman operator theory, have become increasingly prevalent in the analysis of high-dimensional, complex systems. In this presentation I discuss how these methods can be theoretically generalized to handle data related to inputs and control. As a motivating example, these equation-free methods can be applied to the field of epidemiology focusing on the eradication of infectious disease.

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MS146

Operator Theoretic Framework for Estimation and Control

We present a new Koopman operator (KO) theoretic framework for nonlinear model reduction, estimation and optimal control. KO is a linear but an infinite-dimensional operator whose spectral properties can be utilized to transform nonlinear estimation/control problems into a form which facilitates application of techniques developed for linear, Lipschitz or bilinear systems. The proposed framework can be implemented both in a model based and data-driven fashion, and its usefulness will be illustrated though various examples.

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MS147

Inverse Random Source Scattering Problems in Several Dimensions

This talk is concerned with inverse random source scattering problems in several dimensions. The random source is assumed to be driven by an additive white noise. Given the random source, the direct problem is to determine the radiated random wave field. The inverse problem is to reconstruct statistical properties of the random source from the boundary measurement of the radiated random wave field. We show that the direct problem has a unique mild solution by a constructive proof. Using the mild solution, we derive effective Fredholm integral equations to solve the inverse problem. The regularized Kaczmarz algorithm is developed via multi-frequency scattering data to overcome the challenges of solving the ill-posed and large scaled integral equations. Numerical experiments will be presented to demonstrate the efficiency of the proposed method.

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MS147

Acoustic Scattering by a Sphere in the Time Domain

Transient acoustic waves are generated or scattered by a sphere. This leads to initial-boundary value problems for the wave equation. Recent studies usually assume that solutions are smooth. However, many interesting physical problems lead to non-smooth solutions: there are moving wavefronts. These situations are usually handled by seeking weak solutions, but care is needed to ensure that constraints imposed by the underlying continuum mechanics are respected. We investigate some of the consequences.

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MS147

Stekloff Eigenvalues in Inverse Scattering

We consider a problem in non-destructive testing in which small changes in the (possibly complex valued) refractive index $n(x)$ of an inhomogeneous medium of compact support are to be determined from changes in measured far field data due to incident plane waves. The problem is studied by considering a modified far field operator $\mathcal{F}$ whose kernel is the difference of the measured far field pattern due to the scattering object and the far field pattern of an auxiliary scattering problem with the Stekloff boundary condition imposed on the boundary of a domain B where B is either the support of the scattering object or a ball containing the scattering object in its interior. It is shown that $\mathcal{F}$ can be used to determine the Stekloff eigenvalues corresponding to B where if $B \neq D$ the refractive index is set equal to one in $B \setminus \overline{D}$. A formula is obtained relating changes in $n(x)$ to changes in the Stekloff eigenvalues and numerical examples are given showing the effectiveness of determining changes to the refractive index in this way.

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MS147

Fast Computation of 2D-Periodic Green Functions in 3D Near Cutoff Frequencies

We present an efficient method for computing wave scattering by 2D-periodic diffraction gratings in 3D space near cutoff frequencies, at which a Rayleigh wave is at grazing incidence to the grating. At these frequencies (a.k.a. Wood-anomaly frequencies), the lattice sum for the quasi-periodic Green function diverges. We present a modification of this lattice sum that produces algebraic convergence.

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MS148

Modeling Neuronal Electromechanics Using Fractional Operators of Variable Order

Traumatic brain injury (TBI) is among the leading causes of death and permanent disability worldwide. Biomechanical models of TBI existing in the literature do not incorporate either electrochemical or multiscaling features. Since neurons are the brain cells responsible of electrochemical signaling on multiplexed temporal scales we use a constrained Lagrangian formulation and Hamiltons principle to formulate a mathematical model of neuronal electromechanics where the multiple temporal scales are modelled using fractional operators of variable order.

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MS148

Drift-Diffusion Simulation of Channels and Synapses

The drift-diffusion (PoissonNernstPlanck) model is applied to two biological problems: (i) the potassium channel in a biological membrane, and (ii) the triad synapse of the retina. For (i), 2D cylindrically symmetric simulations are presented which show significant boundary layers in the channel. For (ii), the drift-diffusion model with embedded membrane boundary conditions is applied to a realistic 2D cross-section of the triad synapse to verify the existence of strictly electrical (ephaptic) feedback.

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MS148

A Multidomain Electrodiffusion Model of Cortical Spreading Depression

Cortical Spreding Depression (SD) is a slow pathological wave of ionic homeostasis disruption that propagates through the brain. It is thought to be closely related to migraine headache and stroke as well as many other brain pathologies. In this talk, we present a ionic electrodiffusion model of SD taking into account the multi-compartmental nature of brain tissue. We present numerical results showing a successful computation of the change in extracellular voltage during SD, and show how glial parameters shape the details of the SD wave.

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MS148

Models for Tear Film and Ocular Epithelium Interaction

We build on prior models for ion and water transport in corneal epithelial cells by Levin et al. [Invest. Ophthalmol. Vis. Sci. (2006) 47(1):306-316; (2004) 45(12):4423-4432] in order to determine their interaction with the thinning tear film. This work is important since prior studies have hypothesized that epithelial transport is either negligible or important during evaporative thinning of the pre-corneal tear film. We find that the affect on the cells varies with conditions. Supported by NSF DMS 1412085.

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MS149

Numerical Solutions for Fractional Convection Equations

Abstract Not Available at Time of Publication

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MS149

Fractional Boundary Conditions

We address an important open problem in fractional calculus, namely, the formulation of physically meaningful and well-posed boundary value problems for fractional-in-space partial differential equations (FSPDE) on bounded intervals of $\mathbb{R}$. Riemann-Liouville and Caputo-type fractional derivative operators are defined on spaces of functions taking values in the interval $[0, 1]$ whose domains encode combinations of Dirichlet (absorbing) and Neumann-type (no flux) zero boundary conditions. The well-known Grünwald formula is modified using the boundary conditions to obtain Grünwald approximation operators for these fractional derivative operators. Using the theory of semigroups, the well-posedness of the Cauchy problem for FSPDE with boundary conditions is established. In doing so, the stochastic processes associated with these fractional derivative operators are identified as the limits of (sub)-Markov processes associated with the respective Grünwald approximations. Time evolution plots of numerical solutions using Grünwald approximations to FSPDE with boundary conditions will also feature in this talk.

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MS149

Fractional Laplacian and Applications

Abstract Not Available at Time of Publication

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MS149

Second-Order Convergence of Non-Smooth Solutions to Multi-Term Fractional Differential Equations

Abstract Not Available at Time of Publication

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MS150

The XFEM in a Simplified Model for Hydraulic Fracturing in Three Dimensions

In simulations of hydraulic fracturing, three fields are typically involved: the propagation of the crack due to the fluid loading, the fluid flow inside the crack, and the deformation of the surrounding rock based on the XFEM. We propose an approach that consistently works in two and three dimensions and allows for freely propagating cracks which are not not restricted to be planar. The fluid flow is largely simplified by using simple relations between the crack width and the pressure. The crack propagation is based on stress intensity factors that are fitted from crack opening displacements.

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MS150

An XFEM Model for Propagation and Reorientation of Hydraulic Fractures

This talk presents a development of a fluid-coupled algorithm for modeling (i) the propagation of multiple transverse radially symmetric hydraulic fractures from a horizontal wellbore, and (ii) reorientation of longitudinal fractures propagating from a vertical wellbore. Fracture propagation is modeled using the extended finite-element method (XFEM), coupled with a fluid solver based on the Reynolds lubrication equation. To model fracture reorientation, the direction of fracture propagation is determined based on the maximum tensile stress criterion.

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MS150

Meshfree Direct Simulation "Monte Carlo"

Traditional Direct Simulation Monte Carlo (DSMC) approaches resolve collisions by lumping particles within a cell into a single position in space. This introduces an O(h) error, thus limiting the approach to first order in space. In this talk, we present an idea how meshfree techniques (similar to radial basis function) can be employed to improve the local approximation quality, thus providing the potential to conduct DSMC with significantly fewer particles than traditional mesh-based approaches.

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MS150

Modeling of Liquefaction with MPM

Soil liquefaction describes a loss of strength of loose saturated soils upon sudden or cyclic loading. A slight disturbance only might lead to severe damage, e.g. collapse of seadikes or buildings during earthquakes. Modeling of the state transition between saturated soil and a liquefied soil-water mixture is crucial for saturated sandy soils, but forms a numerically challenging problem especially when it involves large deformation processes. In order to simulate the process of liquefaction first an elastoplastic model is integrated with the material point method (MPM) featuring a 2-phase formulation. The MPM allows an accurate description of large deformation problems by combining the advantages of Lagrangian and Eulerian discretizations of the material. In this talk we present first results obtained with this approach for a centrifuge benchmark and discuss the numerical aspects of the simulation for small deformations.

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MS151

Adding Modeling to the Early Undergraduate Engineering Program

Abstract not available at time of Publication

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MS151

Modeling Initiatives for Upper-Level Math Majors: Looking Back, Forward and Across Time Scales

The world around us is multidisciplinary, and modeling lies at the heart of most applications. How does one translate academic knowledge into practical skills? The answer is less than obvious. For some time now GMU Applied Math community has been focusing on training undergraduate math majors to help better prepare them for the modern day interdisciplinary modeling challenges. REU, CSUMS, EXTREEMS and Industrial Modeling workshops are among some of the programs we have developed and run, mentoring over 100 students in the last decade or so. This talk will outline some of the successful strategies and lessons we learned along the way, as well as challenges we encountered. There is clearly a long road ahead.

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MS151

A Zero-Prerequisite Sustainability-Focused Computational Modeling Course for Senior Non-Majors

An experimental course in Environmental Studies at Dartmouth developed three mathematical modules around sustainability-related examples. Modules included lectures, extended computational labs (in pairs), contemporary literature survey, and a substantial final group modeling project. Materials were designed to quickly connect non-math/cs students to quantitative modes of reasoning about familiar problem domains, with an emphasis on rich interdisciplinary critique. The course was well-received. High-level course structure and student-learning goals seem translatable to other application areas.

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MS151

How I Abandoned the Textbook: A Primary Source Driven Modeling Course

Abstract Not Available at Time of Publication

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MS152

Bayesian Multiresolution Modeling of Time to Event Data

We present a flexible family of time-to-event models based on multiresolution hazard (MRH) methodology, a Bayesian semi-parametric approach used for flexible estimation of the hazard rate (and density) together with predictor effects. The method can incorporate non-proportional hazard assumptions, multiple predictors, censoring, reporting delays, and sparsely observed events. We will also introduce MRH, a recently developed R package for multiresolution hazard estimation.

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MS152

A Mathematical Framework for Understanding the Effects of Ecological Interactions on Disease Transmission in Multi-Host Communities

Elucidating the conditions that promote and inhibit transmission of multi-host zoonoses has significance for public health. We developed theory clarifying how competition and contact patterns drive zoonotic disease transmission in multi-species communities. Specifically, we used multi-host compartmental models to compare thresholds for disease emergence in single host species populations vs. multi-host communities. Our approach shows host traits and ecological interactions together determine transmission, and it posits empirically testable mechanisms for disease outbreaks in multi-host communities.

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MS152

Modeling the Dynamics of Human Papillomavirus: Mechanistic Inference from Longitudinal Data

There are over 200 types of human papillomavirus (HPV), the most common sexually-transmitted infection. To understand how variation among HPV types affects the epidemiology, we used Bayesian methods to fit mechanistic models to a longitudinal dataset tracking 37 HPV types that includes information about patient sexual practices. Our results show that the effects of sexual practices on infection risk vary across types, suggesting that strain differences may have complex effects on HPV epidemiology.

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MS152

Survival Analysis of Fall Armyworm in a Tritrophic System through Model Comparison

Understanding how quickly a viral infection spreads through an individual can inform how a disease spreads through a community. In our experimental system, insect herbivores become infected when consuming a lethal virus along with the plant on which the virus resides. Using Bayesian model selection and survival analysis, we provide evidence that an individuals time to death depends upon the interaction between the virus and the plant. Thus, the insects diet governs their survival time.

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MS153

Higher-Order Time-Adaptive Splitting Schemes for Evolution Equations

Many evolution equations can be split into two (or more) parts which separately can be integrated in a simple way. We discuss recent results concerning the analysis and practical application of higher-order splitting schemes. In particular, we address the following topics: - Flexible setup and solution of order conditions for schemes where the right-hand side of the evolution equation is split into two or three parts, - construction of different types of optimized pairs of schemes (similar in spirit to Runge-Kutta pairs), - time-adaptive integration and global error estimation. Some numerical examples will be given for equations of Schrdinger and parabolic types.

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MS153

New Positivity and SSP Analysis of Diagonally Implicit Time-Stepping Methods for PDEs

The most common approach for the construction of positive and SSP methods for time dependent PDEs is based on the Forward Euler (FE) condition for the semidiscretized ODE system. However, there are numerical examples with FEM and WENO5 combined with DIRK methods applied to the advection equations for which the FE condition does not apply but after all the numerical method show positivity and SSP for certain set of step sizes. In this talk we present an analysis of positivty and SSP based on another condition for the analysis which is a generalization of the FE condition and seems more suitable for diagonally implicit general numerical processes (e.g. DIRK, Rosenbrock, W methods) than FE. As a demonstrative application, this new analysis explains the positivity of FEM and WENO5 with DIRK under suitable step size conditions. Optimal methods in some classes of diagonally implicit methods are shown as well.

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MS153

Multilevel Spectral Deferred Correction Methods

I will present recent work on strategies for developing efficient multi-level temporal integration methods based on spectral deferred corrections (SDC). Examples include the embedding of multilevel SDC into block-structured AMR methods and using multiple physical representations on different SDC levels. I will also discuss how multilevel SDC enables parallelization in the time direction through the PFASST algorithm.

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MS153

Building an Efficient Exponential Time Integrator

Exponential time integrators offer an alternative to implicit methods in integrating large stiff systems of differential equations. In this talk we will discuss main theoretical and practical considerations behind building an efficient exponential method. In particular, we will focus on a class of exponential propagation iterative methods of Runge-Kutta-type (EPIRK). We will explain how different classes of EPIRK schemes, such as hybrid, partitioned and implicit-exponential, are constructed and analyzed for given types of problems. A range of numerical experiments of varying degree of stiffness and complexity will be used to illustrate comparative performance of different exponential integrators as well as some implicit methods. In addition, we will present a new software package EPIC that implements the most efficient exponential schemes for serial and parallel computer architectures.

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MS154

Human-in-the-Loop Machine Learning

Data analysis can require immense amounts of data processing, but also requires human insight. When machine learning alone is used to crunch numbers, data stakeholders are left with black-box answers they may not understand or trust. Using visualization for data analysis allows for shifting goals and complex patterns, but misses out on building portable models. I will discuss some work on merging the two approaches, and an outlook on future efforts.

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MS154

Measuring the Effectiveness of Visual Analytics Systems

This talk presents an overview of methods used to evaluate visual analytics systems and technologies. Human-centered performance metrics can help quantify how well a system supports reasoning about data and decision making, but developing and gathering these metrics in controlled ways is often challenging. We explore recent approaches to overcoming typical pitfalls related to evaluating visualizations and visual analytics systems, and present new directions for measuring the effectiveness of these tools.

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MS154

Storytelling with Visual Analytics

Visualization has emerged as a powerful communication medium for data driven insights. As visualization capabilities become more dynamic and more robust, developers are able to mold data into more cohesive, story-like narratives. This talk tracks the development of this technique across the past decade, and delves into the benefits and drawbacks of various approaches.

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MS154

Supporting Bayesian Reasoning in Non-Experts

Decades of research have shown that people perform poorly at estimating and understanding conditional probabilities that are inherent in Bayesian reasoning problems. Yet in the medical domain, both physicians and patients make daily, life-critical judgments based on conditional probability. In this talk, I will discuss the impact of phrasing, visualizations and spatial ability on Bayesian reasoning, and demonstrate how representation can significantly impact the communication of conditional probability in the medical field and beyond.

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MS155

Cubic Regularization for First-Order Methods

Regularization techniques have been used to help existing algorithms solve "difficult" nonlinear optimization problems. Over the last decade, regularization has been proposed to remedy issues with equality constraints and equilibrium constraints, bound Lagrange multipliers, and identify infeasible problems. In this talk, we will focus on the application of cubic regularization in the context of the symmetric rank-one and conjugate gradient methods for nonlinear programming.

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MS155

A Trust-Region Method for Sparse Recovery

In this talk, we consider the $\ell_2 - \ell_p$ sparse recovery problem. We transform this problem into an unconstrained differentiable optimization problem and solve it using a limited-memory BFGS trust-region method. The trust-region method takes advantage of an economical and efficient procedure to obtain a partial spectral decomposition of an L-BFGS matrix. Numerical results suggest that this approach eliminates spurious solutions and is faster than some standard approaches.

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MS155

Manifold Sampling for Nonconvex Piecewise Continuously Differentiable Functions

We present an algorithm for minimizing a continuous, nonconvex mapping of simulation outputs when the derivatives for the simulation, which are assumed to exist, are unavailable. Our trust-region approach builds models of the simulation outputs and includes them in a smooth master model as needed. We show that our algorithm is convergent under reasonable assumptions on the mapping and simulation and then conclude with cases where our techniques are shown to be advantageous in practice.

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MS155

Inexact Alternating Direction Algorithm for Separable Convex Optimization

We introduce inexact alternating direction algorithms with variable stepsize for solving separable convex optimization with linear constraints. Three new methods, called generalized, multistep, and accelerated BOSVS, correspond to different accuracy levels when solving the ADMM subproblems. These algorithms all originate from a 2-block variable stepsize BOSVS scheme, which employs indefinite proximal terms and linearized subproblems. Global convergence and some numerical results will be discussed. This is a joint work with William Hager.

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PP0

PIC Math Student Industrial Math Posters - Presenters To Be Announced

During the spring 2016 semester, mathematical sciences undergraduate students at 50 U.S. universities and colleges were enrolled in a PIC Math (Preparation for Industrial Careers in Mathematical Sciences) industrial mathematics and statistics research course. Each student team worked on a research problem, which came directly from industry, and submitted a written report and video solution to the problem to the PIC Math student research competition. Students will give poster presentations of their research work and solutions PIC Math is a program of the MAA and SIAM supported by NSF funding (DMS-1345499). See http://www.maa.org/picmath

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PP1

Computational Exploration of Integrodifference Population Models

Mathematical modeling of population dynamics can provide novel insight to the growth and dispersal patterns of populations for a variety of species, and has become vital to the preservation of biodiversity on a global-scale. These growth and dispersal stages can be modeled using integrodifference equations that are discrete in time and continuous in space. Previous studies have identified metrics that can determine whether a given species will persist or go extinct under certain model parameters. However, a lack of computational tools necessary to compute these metrics has limited the analysis within many of these studies. We aim to create computational tools necessary to numerically explore a number of associated integrodifference equations, allowing modelers to explore results using a selection of models under a robust parameter set.

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PP1

Uncertainty in Estimating Lead/Lag Relationships

We explore relative glacial termination timings between the eastern and western equatorial Pacific to understand mechanisms of global climate responses to orbital insolation changes. Distributions of the termination timings are estimated using the Bayesian change point algorithm based on age estimates obtained by probabilistic alignment of benthic $\delta^{18}O$ records to a global benthic curve. We conclude that the uncertainties from age estimates and change points are too large to identify any significant lead/lag relationships.

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PP1

Advanced Statistical Learning Algorithms for Comparative Multisource Formation Permeability Modelling

For accurate prediction of formation permeability in noncored intervals, three algorithms were adopted for comparative core permeability modelling given multisource-multiscale measurements of well logs and core data: Shale Volume, Neutron Porosity, Water Saturation, and Rock Lithofacies. The algorithms are Multiple Linear Regression (MLR), Multivariate Adaptive Regression Splines (MARS), and Generalized Boosted Modelling (GBM). GBM has resulted in much more accurate modelling and prediction of formation permeability by achieving the Least Root Mean Square Prediction Error.

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PP1

Parabolic Bursting in Swim CPGs

We study the rhythmogenesis of oscillatory patterns emerging in network motifs composed of inhibitory-coupled parabolic bursters represented by the Plant model of Aplysia-R15 nerve cells. Such motifs are used as building blocks of larger neural networks including central pattern generators (CPGs) controlling swim locomotion of the sea slug Melibe leonine. CPGs are neural networks, which can produce rhythmic activity in isolation. We use alpha synapses to couple the Plant neurons, which are endogenous tonic spikers in isolation.

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PP1

Higher Order Upwind Methods for Maxwell's Equations in Second-Order Form

We present a high-order upwind scheme for the 2D and 3D time-domain Maxwell's equations in second-order form on curvilinear and overlapping grids. The scheme is demonstrated to be stable without the need of additional artificial dissipation usually required by centered finite difference schemes. Stability on overlapping grids is demonstrated by conducting a careful parameter space search to look for unstable solutions. Numerical results confirm the high order of convergence and stability without artificial dissipation.

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PP1

A Multiobjective Optimization for the Performance Measure of EWMA AR (1) Processes When the Observation Is Trend Exponential

In Statistical process control, Exponentially Weighted Moving Average (EWMA) is a well known control scheme. Average run length is one of the most used performance measures for EWMA procedure. In this article, we proposed a Multiobjective optimization approach for the performance measure of EWMA AR(1) processes when the observation is trend exponential.

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PP1

Galerkin Differences: Achieving Very High Order Accuracy Energy Stable PDE Discretizations

We discuss the Galerkin Difference approach to construction of high-order accurate and energy stable difference methods. The technique, based on a Galerkin framework, achieves high order accuracy by including neighboring degrees of freedom (DOFs) into the discretization rather than the more traditional inclusion of interior DOFs. Both theoretical and computational evidence shows that the resulting methods possess excellent dispersion properties. Computational examples demonstrating high-order accuracy for the scalar and elastic wave equations will be presented.

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PP1

Towards Composable Bayesian Inference with PDE Forward Models

We discuss progress towards accelerating and automating the statistical inference of parameters associated with PDE models of physical phenomena. The infrastructure brings together the libMesh parallel adaptive finite element library, the GRINS multiphysics package, and the QUESO statistical library. We discuss how GRINS provides access to modern numerical strategies that facilitate statistical surrogate and MCMC algorithms via QUESO. We show several engineering examples benefiting from the framework at its current stage.

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PP1

The Quilted Synchrosqueezing Transform for

Adaptive Time-Frequency Signal Analysis

The synchrosqueezing transform has recently gained popularity as a tool for sharpening the analysis and mode decomposition of signals with time-varying oscillatory properties. We introduce a synchrosqueezing method based on a *quilted* short-time Fourier transform, where different analysis windows may be chosen to adapt to signal content in different time-frequency regions. We provide theoretical results demonstrating the accuracy of our method, and propose an algorithm for the automatic selection of optimal windows.

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PP1

Numerical Evaluation of Minimum Average Deviance Estimation in Ultra High Dimensional Poisson Regression

The second most expensive part of US Census Bureau's decennial census in 2010 was Address Canvassing (AdCan), a door-to-door data collection in order to update the Master Address File (MAF). The MAF contains important information about all households in the United States. However, the MAF must add and delete addresses every five years based on the habitability of households. Statistical methodologies are being developed to help predict the changes in habitability using a large number of predictors. Adragni et al. proposed a methodology called Minimum Average Deviance Estimation or MADE. It is based on the concept of local regression and embeds a sufficient dimension reduction of the predictors. The goal of this project is to evaluate the performance of MADE on ultra high dimensional data through simulations. The first step is to parallelize several snippets of the MADE R-script in order to help the code run faster and to analyze the speed up of these parallelized snippets compared to their serial alternatives. Simulated data with increasing large dimensions will be used to evaluate the runtime under specified hardware setups. In doing this, a limited stress test will be performed to determine how large of a data set UMBC's High-Performance Computer (HPC), maya, can handle. The results of these tests allow to evaluate the capabilities of MADE which may help the US Census Bureau to predict the additions and deletions to MAF.

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PP1

Unstructured Geometric Multigrid Using PETSc and libMesh

We report progress on the development of an interface between the DM infrastructure in PETSc and the libMesh finite element library to enable linear and nonlinear geometric multigrid-based solvers on unstructured finite element discretizations. In addition, we illustrate performance on prototypical elliptic problems. Finally, we discuss how these developments will enable the use of multigrid-based algorithms on complex multiphysics problems through packages such a GRINS, a recent multiphysics FEM platform built on libMesh.

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PP1

Determining Optimal Economic Policy to Mitigate Catastrophic Loss

A team of civil engineers and economists at several universities recently received a NIST grant to combine catastrophe models from engineering with economic models to produce a tool to be used by policy-makers in determining optimal economic policies to mitigate future disasters. This poster focuses on one piece of this much larger puzzle, namely the development of nonlinear optimization routines to find economic equilibria after a shock.

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PP1

Partial Synchronization in Pulse-Coupled Oscillator Networks

We study N identical integrate-and-fire oscillators coupled through α-function pulses in an all-to-all network. Beyond the traditionally studied, sync and splay states, we find a rich set of other partially synchronized attractors, such as $(N-1,1)$ fixed states and partially synchronized splay states. We develop a dimensional reduction framework in which the pulsed dynamics reduces to a continuous flow, whose direction is the sign of the coupling strength K. Our analytic analysis is complemented with high-precision numerical simulations. We present the bifurcations and the stability of all attractors and limit cycles for $N = 2, 3, 4$.

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PP1

A Stable Algorithm for Divergence and Curl-Free Radial Basis Functions in the Flat Limit

The general method used for calculating smooth RBF interpolants in the flat limit becomes numerically unstable. The RBF-QR algorithm bypasses this ill-conditioning using a clever change of basis technique. We extend this method for computing interpolants involving matrix-valued kernels, specifically divergence-free and curl-free RBFs, in the flat limit. Results illustrating the effectiveness of this algorithm are presented as well as applications to computing the Helmholtz-Hodge decomposition of a vector field from samples at scattered points.

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PP1

Modeling Viscoelastic Flows Through Porous Media

Flow of viscoelastic fluids through porous media has widespread applications in industrial and natural processes. Yet, there is no universally accepted mathematical model for such flows. We will present a macroscale viscoelastic flow model in porous media and provide insights for its extension into multiphase, multicomponent flows associated with chemical EOR methods. Work on this project is currently under progress and preliminary numerical results for single-phase flow will be discussed.

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PP1

An Analysis of Joint Inversion for Regularization of Ill-posed Problems

Joint inversion is technique frequently applied to problems in the physical sciences. It can improve the conditioning of a problem as well as the accuracy of the inverse solutions. We present a mathematical analysis of joint inversion in regard to the regularization of ill-conditioned problems in geophysical electromagnetic imaging. The discrete linear case is examined most thoroughly as it provides the foundation for non-linear problems to be solved iteratively.

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PP1

Node Diversification in Complex Networks by Decentralized Coloring

Graph coloring is a ubiquitous problem in computer science and cyber security. Because of the inherent hardness of the problem, proper coloring requires many colors. However, there are application settings of security by diversity where colors (OS, implementations, functions, etc.) are very expensive to obtain. This motivates the concept of defective coloring (DC) where the two end nodes of some edges are allow to share same color. This setting calls for the DC algorithms that can achieve the best diversity with respect to a small number of colors. In this project we investigate a decentralized DC algorithm and characterizes its power and limitation.

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PP1

Advanced Time Integration Methods for Atmospheric Physics

Global climate models are complex multiscale multiphysics systems encompassing a broad set of processes. Within the Community Atmosphere Model, parameterized subgrid scale column physics processes are sequentially or parallel split in time from one another. Time split couplings can suffer from low accuracy (less than first order) and may lead to instabilities. We introduce the use of Implicit-Explicit (IMEX) integrators to improve process coupling and reduce time stepping errors for atmospheric physics. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-681478

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PP1

Numerical Solutions to the Navier-Stokes Equations with a Free Surface Using Universal Meshes

We introduce a high-order finite element method for the simulation of free-surface flow with surface tension. We discretize the fluid domain using a universal mesh: a background mesh that conforms to the geometry of the free surface at all times by perturbing a small number of nodes in the mesh. The method provides a sharp representation of the free surface, easily handles large deformations, and achieves high-order convergence rates.

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PP1

Resilience Analysis for Multigrid Methods

We present a framework for the analysis of linear iterative methods in fault-prone environments such as next-generation HPC systems. The effects of failures are taken into account through a probabilistic model involving random diagonal matrices. Using this model, we analyze the behavior of two- and multigrid methods under random node failures. Our results show that while standard multigrid is not resilient, protecting the prolongation leads to a fault-resilient variant.

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PP1

Enstrophy Dissipation in 2D Incompressible Flow Via Singular Vortex Dynamics

The enstrophy dissipation in the zero viscous limit is a remarkable property to characterize 2D turbulent flows. However, it is shown that the dissipation never occurs in 2D Euler equations for the function space in which 2D Euler equations have the solvability. Then, we consider a dispersive regularization of Euler equations, known as Euler-α equations. We prove the existence of solutions that dissipate the enstrophy in the $\alpha \to 0$ limit and the dissipation is caused by the singular vortex dynamics.

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PP1

The Dynamics of a Viscoelastic Filament During a Stretch and Hold Experiment

We present the dynamics of a stretch and hold experiment for a filament modeled by the partially extending strand convection model of Larson with a Newtonian solvent. The initial value problem is a cylindrical filament held between two ends, and stretched upward by the top boundary for an interval of time. The top is held and the ensuing dynamics of the filament is described up to pinch-off. We focus on the condition of a small parameter, the ratio of the retardation time to the relaxation time. The filament displays thixotropic yield stress behavior as a result of our assumptions.

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PP1

A Sampling Kaczmarz-Motzkin Algorithm for Linear Feasibility

We combine two algorithmic techniques for solving systems of linear inequalities, the relaxation method of Agmon, Motzkin et al. and the randomized Kaczmarz method. In doing so, we obtain a family of algorithms that generalize and extend both techniques. While we prove similar convergence results, our computational experiments show our algorithms often vastly outperform the original methods.

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PP1

Computing Sobol' Indices for Stochastic Models

Sobol indices are used extensively for global sensitivity analysis of deterministic models. However, stochastic models are replacing their deterministic counterparts in many applications. Generalizing Sobol indices to stochastic models poses both theoretical and computational challenges. We provide a theoretical framework to define the stochastic Sobol indices and present an efficient method for their computation. Preliminary error analysis is given and numerical results presented showing the efficiency and value of our proposed method.

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PP1

New Independent Potentials for the Stationary Klein-Gordon Equation in Terms of the Heun Functions

We present in total thirty-five potentials for which the stationary Klein-Gordon equation is solvable in terms of the general Heun functions and fifteen potentials for which the stationary Klein-Gordon equation is solvable in terms of the confluent Heun functions. Because of the symmetry of the Heun equations with respect to the transposition of their regular singularities, only eleven of the general Heun and nine of the confluent Heun potentials are independent.

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PP1

Comparative Multivariate Rock Lithofacies Classifications Through Multinomial Logistic Regression and Probabilistic Neural Networks

Well logs interpretations of neutron porosity, shale volume, and water saturation, were modeled to estimate the discrete and posterior Lithofacies distributions in sandstone oil reservoirs. The measured Lithofacies sequences were comparatively modeled through Multinomial Logistic Regression (MultiLogit) and Probabilistic Neural Networks (PNN). To assess the prediction accuracy, total correct percent of the predicted discrete lithofacies distributions were conducted for MultiLogit and PNN algorithms. PNN led to more accurate prediction than MultiLogit for its nonlinearity classification.

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PP1

An Energy Conservative, Skew-Symmetric Method for Compressible Flow with Adaptive Mesh Refinement and Fluid-Structure Interaction

A skew-symmetric convective scheme is utilized in conjunction with a collocated tensor discretization (ensuring simultaneous consistency of the total, internal, and kinetic energy equations) in the context of structured adaptive mesh refinement. This allows for long-time stable simulations free from numerical dissipation. The fluid dynamics method is coupled to a novel multi-level scheme for simulating fluid-structure interaction, allowing for non-uniform resolution of the solid body.

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PP1

Generalized Gossip-Based Subgradient Method for Distributed Optimization

This talk introduces a novel optimization method for distributed optimization problems based on the subgradient approach and the generalized-gossip protocol. The proposed method achieves the spectrum from globally optimal solution to locally optimal solution by introducing a user-defined control parameter. The convergence analysis shows the convergence rate and a practice use case is presented to validate the proposed method. This method also shows the potential of isolating faults by use of state transition matrix.

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PP1

Managing the Spread of Alfalfa Stem Nematodes (Ditylenchus Dipsaci): The Relationship Between Crop Rotation Periods and Pest Re-Emergence

In the western US, alfalfa crops affected by stem nematodes (Ditylenchus dipsaci) are prevalent. Understanding dynamics associated with this pest will lead to better management programs. I present a host-parasite model that portrays a relationship between the crop rotation duration and the time at which the density of nematode-infested plants becomes larger than that of healthy ones in the post-rotation alfalfa. Numerical results suggest the model could play a role in improving crop management strategies.

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PP1

Collegiate Leadership Development: Analyzing Data from the Multi-Institutional Study of Leadership

We have data from Virginia Tech's participation in the 2015 Multi-institutional Study of Leadership, including survey responses from 1,686 students. There are 500+ variables to analyze, including questions about leadership efficacy, socially responsible leadership, social perspective-taking, mentoring relationships, academic college experiences, formal leadership training experience, community service involvement, etc. MSL emerged to specifically address questions regarding students educational needs and to identify elements of the higher education environment that contributed most significantly to leadership outcomes.

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PP1

Study on the Viscoelastic Fluid Flows using Adaptive Least-Squares Finite Element Methods

The work concerns least-squares finite element solutions of viscoelastic fluid flows using adaptively refined grids. Model problem considered is the flow past an transverse slot problem. Results of the adaptive refined meshes generated by the stress are presented, along with comparisons using a velocity gradient refinement for the least-squares functional. Numerical results indicate that the refinement results of the stress are effective for analyzing viscoelastic fluid flows.

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PP1

Parameter Estimation, Ill-Conditioning and Identifiability Analysis of the Anaerobic Digestion Model No 1 (adm1) for Biogas Production

The biogas production using anaerobic processes has recently received worldwide attention as alternative energy. The ADM1 is a first-principles model considering biochemical and physicochemical processes. Although its parameterization has been addressed in several researches and its identifiability problems are well-recognized, there no exist so far any study to systematically analyze its possibly ill-conditioning and its effects on identifiability and parameter uncertainty. Our aim is to investigate how the available experimental data impact on these aspects.

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PP1

Image Deblurring with Blur Learning

Image clarity is important for a variety of applications such as navigation, medical imaging, and space exploration. Unfortunately, every image is blurred to some extent due to instrument error, camera motion, or the environment (e.g. atmospheric turbulence). Recent deblurring techniques leverage sparsity of natural images in transform domains such as wavelets. However, many of these techniques assume that the blur is known, which is a significant limitation. We present an algorithm that simultaneously updates the blur while recovering the true image.

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PP1

A Stable and Efficient Interface Condition for Conjugate Heat Transfer Problems

We developed new partitioned coupling conditions for conjugate heat transfer problems. The method introduces no explicit grid overlap and exhibits similar characteristics to the Dirichlet-Neumann approach when the thermal conductivity and diffusivity in subdomains are greatly different (i.e. rapid convergence). In addition, this new method also converges rapidly in the problem where the coefficients in subdomains are close or identical. The algorithm is constructed using a Robin condition with optimal weights similar to the construction of optimal Swartz methods for domain decomposition.

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PP1

Runge-Kutta-Chebyshev Time Stepping for Parabolic Equations on Adaptively Refined, Quadtree Meshes

We show progress towards developing an explicit Runge-Kutta-Chebyshev (RKC) time stepping method for multirate time stepping on adaptively refined, Cartesian meshes. Central to our investigation will be to show that RKC time stepping can be done efficiently and is competitive with standard implicit methods for parabolic equations. We show results in 1D, but eventually will incorporate RKC time stepping into ForestClaw, a library for solving PDEs on adaptively refined, multi-block quadtree meshes.

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PP1

Bayesian Global Optimization of Noisy Functions

We propose an extension to Bayesian global optimization suitable for noisy expensive objectives without gradient information. Such objectives arise from stochastic simulations, e.g. models with parametric uncertainties, molecular dynamics simulations, or experiments. Our approach is based on a Bayesian surrogate that estimates the measurement noise and on a modified version of the expected improvement. The ability, to quantify the epistemic uncertainties that arise due to limited data, is exploited to derive stopping criteria.

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PP1

Quantitative Estimates in Nonlinear Elasticity

A deformation $u : U \to \mathbb{R}^n$ of an elastic body can be approximated by a rigid motion $Ax + c$ according to an estimate of R. Kohn

$$\int_U |u - (Ax + c)|^2 dx \leq C \int_U |e(Du)|^2 dx$$

where $e(Du)$ is computed from invariants of the Cauchy-Green tensor. We study a quantitative variant of the estimate.

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PP1

Dynamical Analysis of Connected Neuronal Motifs with OpenAcc and OpenMPI

Large scale analysis of the dynamical behavior of Central Pattern Generators(CPGs) formed by neuronal networks of even small sizes is computationally intensive and grows exponentially with network size. We have developed a suite of tools to exhaustively study the behavior of such networks on modern GPGPU accelerators using the directive based approach of OpenAcc. We also achieve parallelization across clusters of such machines using OpenMPI. Directive based approaches simplify the task of porting serial code onto GPUs, without the necessity for expertise in lower level approaches to GPU programming, such as CUDA and OpenCL. 3-cell neuronal CPGs have been explored previously using various GPGPU tools [1]. As motifs form the building blocks of larger networks, we have employed our framework to study 4-cell CPGS and two connected 3-cell motifs. We discuss the performance improvements achieved using this framework and present some of our results.

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PP1

Dissipative Particle Dynamics Simulation of Polymer Nanomaterials for Drugs Delivery

Input your abstract, including TeX commands, here. Mesoscale scale dissipative Particle Dynamics (DPD) link the disruption between molecular dynamics and continuum mechanics. Here we trekked dissipative particle dynamics (DPD) and coarse-grained molecular dynamics of polymernanomaterial-drug interfaces to understand the encapsulation and bioavailability of various cancer drugs. Drug encapsulation and efficient drug delivery is usually achieved by expensive and arduous experiments. To increase the promptness choosing excipient are also very tedious process. Many carrier fluid such as tristearin, glyceryl behenate bilayer lipid carrier SLM without alcohol, cellulose, PEG, dendrimers, surfactants are used as carriers for guest species in various pharmaceutical applications. DPD simulations are compared with available experimental data, which showed good correlation in the presence of certain composition of polymer and nanomaterial with selected drugs. DPD simulations also revealed certain hydrophobic/hydrophilic drugs interactions under certain conditions. In this presentation we will explore the drug interaction and encapsulation efficiency via DPD and coarse grained techniques.

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PP1

The Role of the Replacement Rate in the Basic Reproduction Number

The basic reproduction number, defined as the number of secondary infections produced by an infected individual in a homogeneous susceptible population, is a fundamental concept in epidemiology. In models with gamma-distributed transitions, the basic reproduction number is independent of the number of compartments if there is no replacement, but depends on the number of compartments when replacement is introduced. We investigate this effect and explore the mechanisms relating basic reproduction number and replacement rate.

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PP1

Eigensurfaces of Reflectors and the Passenger Side Mirror Problem

We consider surfaces that remain invariant up to scaling when viewed in a curved reflector. Such “eigensurfaces” always exist in the rotationally symmetric case, but not in general. However, if one views both reflector and eigensurface as unknown, then one may use a finite difference method to find a solution pair. One application is to find a reflector that gives a scaled view of a plane, which gives a wide-angle, non-distorting passenger side mirror.

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PP1

Development of Integer Programming Models for LCD Mother Glass Manufacturing As a Two-

Dimensional Strip Packing Problem

Process industries are under heavy pressure to reduce the loss from the operation. The minimizing the loss contributes to improve the process efficiency and profitability in the end. As many process operations are automated, rigorous systematic efforts should be developed instead of previous manual based heuristic operations. This paper illustrates such an effort in the context of LCD glass manufacturing. Particularly an integer programming model for minimizing the loss generated in cutting LCD glass is proposed in this paper. The main concept of the proposed model is to minimize the strip denoting the length of the large rectangle, used to pack multiple demands of small sizes. Numerical case studies from an actual LCD manufacturing company are presented to illustrate the applicability of the proposed model with some remarks.

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PP1

Sufficient Conditions for Stability of Permanent Rotations of a Two-Gyrostat Chain in a Central Gravitational Field

In this contribution we establish and analyze sufficient conditions for stability of permanent rotations of a chain that consists of two Lagrange gyrostats and moves about a fixed point under the action of a central gravitational force. Our findings extend corresponding results in the dynamics of a single gyrostat to a case of the multibody chain as well as generalize some of the known properties of permanent rotations in the many-body dynamics.

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PP1

Effects of Auxiliary Information on Ewma Control Chart

The efficiency of EWMA chart in monitoring location parameter can be improved by using auxiliary variable. We propose a new EWMA-type structure using ratio estimator to increase its efficiency in monitoring location parameter, and it is shown that it outperform its existing counterparts, especially when there is a strong positive relationship between the variable of interest and the auxiliary variable. The proposed charts performance is measured using ARL, SDRL, EQL, RARL, and PCI.

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PP1

Blind Reconstruction of a Single-Source Signal Embedded in Another Signal

This paper investigates a blind reconstruction model of single-source signal and another signal which is on an unknown wall and covers source signals. The main purpose is to separate the source signal from mixed observed signals. We construct a mathematical formula and conduct numerical experiments on the assumption that the observed data are known, while the others data are unknown. Fairy good results are obtained with respect to the source separation and unknown data reconstruction.

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PP1

Effects of Biodiversity on Epizootics: The Importance of Decreasing Variability in Transmission

Empirical and theoretical research has demonstrated that increasing host biodiversity decreases disease transmission, known as the dilution effect. This effect, however, only considers changes in the mean transmission rate, not the variability associated with transmission. By combining statistical and mathematical models with data, we examine how increased biodiversity in a tri-trophic system can lead to more consistent outcomes. Thus the dilution effect may be driven by changes in the mean and the variability of transmission.

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PP1

Generalization of Arithmetic Progression and Sums of Powers

In arithmetic progression (A.P) series general formula, the values of the first term and common difference can be varied but with the terms powers fixed. In sums of powers it is vice versa. This research aims at finding a general formula for both A.P series and sums of powers. Using Mathematical Induction and analytic number theory methods, the general formula was formulated. The new formula closes the gap between A.P series and sums of powers.

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PP1

Optimal Mating Strategies for Simultaneous Hermaphrodites in the Presence of Predators

Certain preferentially outcrossing simultaneous hermaphrodites are capable of self-fertilization. While self-reproducing organisms transmit two sets of genes to offspring, often inbreeding depression leaves outcrossing the better strategy. The accepted model to optimize self-reproductive delay fails to account for certain organisms response to predators. In this poster, we discuss the theoretical implications of incorporating this response, including life history scenarios and the existence of hysteresis, the lack of reversibility as a parameter is varied.

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PP1

Tsunami Sediment Transport with GeoClawSed

GeoClawSed is based on GeoClaw and adds a bed updating and avalanching scheme to the two-dimensional coupled system combining the shallow water equations and advection-diffusion equation. GeoClawSed can evolve different resolution and accurately capture discontinuities in both flow dynamic and sediment transport. GeoClawSed is designed for modeling tsunami propagation, inundation, sediment transport and topography change. The model presented is tested by 2011 Tohoku-oki Tsunami in Sendai airport area with sediment data got from field survey.

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PP1

Trace Theorems for Some Nonlocal Function Spaces

It is a classical result of Sobolev spaces that any H^1 function has a well-defined $H^{1/2}$ trace on the boundary of a domain with sufficient regularity. In this work, we present some nonlocal generalizations of such a trace theorem in new function spaces that contain the classical H^1 space as a subspace. The new spaces are associated with nonlocal norms that are characterized by nonlocal interaction kernels defined heterogeneously with a special localization feature on the boundary. We show that the $H^{1/2}$ norm of the trace on the boundary is controlled by these nonlocal norms that are weaker than the classical H^1 norm. These results are improvement and refinement of the classical results since the boundary trace can be attained without imposing regularity of the function in the interior of the domain.

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PP1

Stable and High-Order Accurate Finite Difference Methods for the Wave Equation with Non-Conforming Grid Interfaces

We present a new result on using high-order finite difference methods to solve the wave equation in the second order form. Particular emphasis is placed on the numerical treatment of non-conforming grid interfaces with hanging nodes. The highlight of the proposed numerical scheme is that it is provably stable. We also verify its high accuracy in numerical experiments.

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PP1

Spectra of Quantum Trees and Orthogonal Polynomials

This study concerns the asymptotic spectrum of quantum trees as their diameter becomes unbounded. A quantum tree is a connected graph with no cycles together with a Schrödinger operator on each edge and self-adjoint vertex conditions. We prove that the eigenvalues of a sequence of quantum trees are the roots of a sequence of orthogonal polynomials. The limiting density of eigenvalues is studied through the asymptotic theory of orthogonal polynomials.

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PP1

Goal-Oriented Network Design for Pairwise Comparison Ranking

Consider a collection of items with some unknown but intrinsic ordering and incomplete noisy pairwise comparison data. How can the ranking of the items be inferred with additional data? We address this interesting problem by designing goal-oriented comparison networks which allows for efficient additional data collection that yield enhanced ranking reconstruction. We benchmark our network design approach using synthetic models, and also show applications to several real-world datasets.

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PP1

Multigrid Framework for Multiphysics Problems

The implicit solution of multiphysics problems plays an increasingly important role in many engineering applications. Modern monolithic multigrid preconditioners often outperform traditional methods as they solve the involved physical and mathematical fields simultaneously while considering the coupling of the solution variables on all multigrid levels. We present a new flexible multigrid software framework for multiphysics problems which facilitates the incorporation of state-of-the-art components within a multilevel preconditioner and minimizes the implementation effort for application-specific extensions.

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PP1

Lagrangian Data Assimilation of Traffic-Flow Models

Our goal is to apply data assimilation techniques to microscopic and macroscopic traffic models to estimate traffic states and parameters. We found ways in which sensor data as well as GPS data of moving cars can be assimilated in a unified freeway. We implemented this approach using both ensemble Kalman and particle filter and evaluated their efficacy using micro and macro models. We applied our results to real traffic data from Minnesota Transportation Department.

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PP1

Online Adaptive Model Reduction for Flows in Heterogeneous Porous Media

We propose an online adaptive model reduction method for flows in heterogeneous porous media. Our approach constructs a reduced system by proper orthogonal decomposition (POD) Galerkin and the discrete empirical interpolation method (DEIM). Moreover, we adapt the reduced system online by changing the reduced solution space and the DEIM approximation of the nonlinear functions. The online adaptation incorporates new data becoming available online to yield a reduced system that accurately approximates dynamics not anticipated in the offline stage.

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PP1

Stiffness of the Arched Human Foot

Curved elastic shells are substantially stiffer than flat plates, because out-of-plane bending is coupled to in-plane stretching. We hypothesize a similar mechanism in the human foot, where the transverse arch induces a bending-stretching coupling. Direct measurement of human foot stiffness is however beyond current measurement techniques. Motivated by simple models of the foot, we design human subject experiments that test this hypothesis without the need for direct stiffness measurements.

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PP1

Decision Analysis for Water-Energy Nexus Considering Multiple Objectives

In energy-water nexus management, multiple conflicting objectives exist. A multi-objective energy-water nexus optimization model is thus developed coupled with sensitivity and decision optimization tools provided by MADS (http://mads.lanl.gov). The model is capable to quantitatively identify the tradeoffs among multiple conflictive objectives in energy-water nexus management, and is tested in a synthetic problem. Different solutions for energy-water nexus strategies can be obtained for addressing the preferences of decision makers on different management objectives.

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PP2

AWM Workshop: A Multi-Risk Model for Understanding the Spread of Chlamydia

Chlamydia trachomatis, Ct, infection is the most frequently reported sexually transmitted infection in the United States. To better understand the recent increase in disease incidence, and help guide in mitigation efforts, we created and analyzed a multi-risk model for the spread of chlamydia in the heterosexual community. The model incorporates the heterogeneous mixing between men and women with different numbers of partners and the parameters are defined to approximate the disease transmission in the 15-25 year-old New Orleans African American community. We use sensitivity analysis to assess the relative impact of different levels of screening interventions and behavior changes on the basic reproduction number. Our results quantify, and validate, the impact that reducing the probability of transmission per sexual contact, such as using prophylactic condoms, can have on Ct prevalence.

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PP2

AWM Workshop: Modeling of Mrna Localization in Xenopus Egg Cells

mRNA localization is essential for Xenopus egg and embryo development. This accumulation of RNA at the cell periphery is not well understood, but is thought to depend on diffusion, bidirectional movement and anchoring mechanisms. Our goal is to test these proposed mechanisms using partial differential equations models and analysis, informed by parameter estimation. Our results confirm that diffusion coefficients and transport speeds are different in various regions of the cell cytoplasm.

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PP2

AWM Workshop: Fitness Effects of Defense Strategies on Plants under Herbivory

Abstract: When attacked by insect herbivores, plants emit volatile chemicals. These chemicals are known to induce local defenses, prime neighboring plants for defense, and attract predators and parasitoids to combat the herbivores, but these chemical defenses are coupled with fitness costs. We examine the interactions between the model plant goldenrod and one of its insect herbivores, Trirhabda virgata, in order to explore how a plants defense strategy can increase or decrease its fitness.

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PP2

AWM Workshop: Quantifying Dynamic Growing Roots in 3D by Persistent Homology

Quantifying changes in root architecture, as a function of growth and environmental interactions constitutes a major challenge and emerging frontier in plant biology. Persistent homology is a powerful topological data analysis technique that holds great promise for modeling and quantifying variation in complex shapes. Starting with existing 4D root data, we develop technique based on persistent homology to analyze variation of root form and shape during growth and to investigate size-shape developmental constraints.

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PP2

AWM Workshop: A Numerical Investigation of a Simplied Human Birth Model

We explore the effects of fetal velocity and fluid viscosity on the forces associated with human birth. The numerical model represents the fetus moving through the birth canal using a rigid cylinder that moves at a constant velocity through a passive elastic tube (modeled by a network of springs) immersed in viscous fluid. The Stokes equations, solved with the method of regularized Stokeslets, describe the relationship between velocity and forces in the system.

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PP2

AWM Workshop: Identification of the Vasodilatory Stimulus from Cerebral Blood Flow Data

A localized increase in neural activity is accompanied by a significant increase in cerebral blood flow (CBF) and cerebral blood volume (CBV) in the surrounding brain tissue, a process known as functional hyperemia. Existing mathematical models that explain functional hyperemia following a vasodilatory stimulus assume that the stimulus is known. Rather than modeling the hemodynamic response as a system of differential algebraic equations, we reformulate the model as an inverse problem, using CBF data to find the underlying stimulus. This results in accurate estimates of the vasodilatory stimulus, its vascular location, and the underlying blood flows and blood volumes of the system.

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PP2

AWM Workshop: Littles Law Applied to a Stochastic Model of Poliomyelitis

Poliomyelitis is an infectious disease that is currently endemic in regions such as Afghanistan and Pakistan. The oral poliovirus vaccine (OPV) is an attenuated form of the virus that is used to prevent polio in these endemic regions. OPV is contagious, so it can provide herd immunity. A disadvantage is that OPV can cause paralysis and is no longer used in many countries. The main concern in regards to the eradication of polio is the silent circulation. After an individual has had an initial contact with the virus, whether through infection or vaccination, the individual will be asymptomatic after any subsequent infection with the virus. We want to answer the following question. In a community of individuals whose immunity to poliovirus has waned, how long can the silent circulation persist? We developed a stochastic model to analyze the silent circulation.

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PP2

AWM Workshop: Diffusion Maps for Image Segmentation

Efficient representation of high dimensional data is an active area of research. We present our solution by introducing diffusion maps as a way to achieve a faithful Fourier-like representation of the data. This method will only need the assumption that data lives on or close to a manifold, and will be able to detect intrinsic features. While this approach can be used for different purposes on data, we will apply it for image segmentation purposes.

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PP2

AWM Workshop: Modeling Cooperation and Competition

Sympatric speciation is a complex phenomenon which is not yet well understood. In my research I am examining sympatric speciation arising from cooperation. I am investigating how a single population of generalists or noncooperators might then evolve into two populations of cooperating specialists to an extent that the different cooperators are considered different species. In working to model this occurrence I used systems of ordinary differential equations, adaptive dynamics, and numerical simulations.

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PP2

AWM Workshop: A Multi-Scale Model of Escherichia Coli Chemotaxis from Intracellular Signaling Pathway to Motility and Nutrient Uptake in Nutrient Gradient and Isotropic Fluid Environments

We present a multi-scale mathematical model of Escherichia coli chemotaxis in a fluid environment that links the biochemical dynamics of intracellular signaling and flagellar dynamics to the behavior of cells and the surrounding nutrients and fluid flow. The resulting feedback between hydrodynamics and chemotaxis not only shows expected run and tumble behaviors of bacterial cells but also depicts the importance of fluid dynamical effects on the transport and consumption of chemoeffectors.

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PP2

AWM Workshop: Online Adaptive Model Reduction for Flows in Heterogeneous Porous Media

We propose an online adaptive model reduction method for flows in heterogeneous porous media. Our approach constructs a reduced system by proper orthogonal decomposition (POD) Galerkin and the discrete empirical interpolation method (DEIM). Moreover, we adapt the reduced system online by changing the reduced solution space and the DEIM approximation of the nonlinear functions. The online adaptation incorporates new data becoming available online to yield a reduced system that accurately approximates dynamics not anticipated in the offline stage.

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PP2

AWM Workshop: Artificial Diffusion Limiters for Discontinuous Galerkin Methods Solving Hyper Bolic Conservation Laws

We investigate a new limiting approach based on previous WENO limiters for discontinuous Galerkin methods solving nonlinear conservation laws. The idea is to add an artificial viscosity term containing the difference between the numerical solution and the reconstructed polynomial, to the original formulation of the DG method. The new approach can control oscillations near discontinuities without sacrificing accuracy, while converge correctly for steady state problems. Numerical results are provided to illustrate the performance.

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PP3

A Dispersion Minimized Mimetic Finite Difference Method for Maxwells Equations in Linear Dispersive Dielectrics

We present a mimetic method for Maxwell's equations in linear dispersive media in which the macroscopic electric polarization is modeled by a system of ordinary differential equations forced by the electric field. An optimization process called m-adaptation along with exponential time differencing is used to construct a method based on edge discretizations in space and mass lumping that has fourth order numerical dispersion in its stable range.

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PP3

Modeling and Detecting Arcs in Magnetohydrodynamic Generator Channels

Magnetohydrodynamic power generators extract electrical power from an ionized gases by passing it through a strong magnetic field. While theoretically very efficient, this technique suffers from material failures caused in part by arcing. We aim to estimate the location of arcs from perturbations of the magnetic field. We model the system with partial differential equations and introduce an artificial conductivity profile as a heuristic. We present the model, sensitivity studies, and a inverse problem methodology.

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PP3

Operator Splitting Methods for Maxwell's Equations in Ferromagnetic Materials

We present operator splitting methods for the 3D Maxwell's equations in a ferromagnetic material in which the magnetization is modeled using the Landau Lifschitz Gilbert (LLG) model from micromagnetism. We present an analysis of our splitting methods for the Maxwell-LLG system and results of numerical simulations that illustrate the theoretical results.

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PP4

Randomized Methods for Matrix Estimation in Inversion, Optimization, and UQ

We analyze randomized methods to reduce the costs of large-scale inversion, optimal design, and uncertainty quantification.

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PP4

Computing the Matrix Logarithm at Higher Precision

We present a multiprecision algorithm to compute the principal logarithm of a matrix to arbitrary precision, given multiprecision arithmetic. Our approach combines the well established inverse scaling and squaring method with an improved version of the classical bound for the error of Pad approximation of Kenney and Laub, which is sharper for highly nonnormal matrices. We compare the behaviour in high precision of truncated Taylor series and diagonal Pad approximants.

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PP4

Network Asymmetry Through Time Dependency

Given a single network of interactions, asymmetry arises when the links are *directed*. A different type of imbalance can arise when interactions appear and disappear over

time. If A meets B today and B meets C tomorrow, then (in the absence of any further relationships between them) A may pass a message or disease to C, but not vice versa. I will describe and illustrate a new algorithm that quantifies this type of temporal asymmetry.

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PP4

Estimating the Largest Elements of a Matrix

We derive an algorithm for estimating the largest $p \geq 1$ elements of an $m \times n$ matrix A, along with their locations in the matrix. The matrix is accessed using only matrix–vector or matrix–matrix products. The algorithm iterates on $n \times t$ matrices, where $t \geq p$ is a parameter. For $p = t = 1$ we show that the algorithm is essentially equivalent to rook pivoting in Gaussian elimination and we obtain a bound for the expected number of matrix–vector products. For $p > 1$ we incorporate deflation to improve the performance of the algorithm. Experiments on both artificial and real-life datasets show that the algorithm provides excellent estimates. In particular, it can identify the largest elements of matrices defined implicitly as A^TA or e^A, for large, sparse matrices A, thousands of times faster than if these matrices were explicitly formed.

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PP4

Recent Developments Within the Feast Eigenvalue Solver

The current release of the FEAST Eigensolver (v3.0) supports non-Hermitian eigenproblems. New routines have been added (and optimized) for the complex symmetric, complex non-symmetric, and real non-symmetric matrix cases. Current directions are targeting a fully parallel version of the software with three distinct levels of MPI parallelism and allow the main computational task, solving a set of linear-systems, to be performed with a distributed-memory solver. Examples are presented using MKL cluster pardiso, SPIKE-MPI, and domain decomposition solvers.

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PP4

Hierarchical Computations on Manycore Architectures (hicma)

At extreme scale, fast multipole and closely related H-matrix methods may dominate in solving many linear systems arising from differential and integral equations, statistics, and machine learning – possessing a combination of low arithmetic complexity, high arithmetic intensity, low communication complexity, and potential for relaxed synchrony. They are, however, complex to implement efficiently on SIMT-like hardware, which is the goal of the HiCMA project at KAUST. We report on work leading to such "HBLAS for accelerators.'

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PP4

Uncovering Hidden Block Structure

We describe a multistep procedure for uncovering block structure in a matrix. In this work we combine standard combinatorial techniques with a novel clustering technique that combines numerical and structural analysis using properties of the SVD of a doubly stochastic matrix. Our algorithm requires no prior knowledge of any structure and can be used to cluster and as a partitioning scheme in preconditioning and block iterative methods.

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PP4

High-Performance Right-Looking Householder-Based LLL and BKZ (2.0)

Despite the numerous applications of lattice reduction (e.g., in algebraic number theory and lattice-based cryptography) and the close connection between the Lenstra-Lenstra-Lovasz (LLL) algorithm and column-pivoted QR factorizations (through generalizing from permutations to unimodular transforms), the well-established techniques for exploiting level 3 BLAS within Householder QR have not yet been extended. We therefore propose a novel right-looking variant of a Householder-based (modified, deep-insertion) LLL which both accumulates Householder transformations where possible and avoids redundant applications when the Lovasz condition requires column swaps. We provide benchmarks of the new scheme, a tree-based, recursive extension, and its embedding within BKZ (2.0), against the corresponding implementations from the popular NTL and FPLLL libraries.

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PP4

Computing a Random Eigenvalue Distribution by Solving a PDE

The Tracy-Widom distribution is one of the most important distributions in random matrix theory, governing the behavior of the largest eigenvalue for a broad class of random Hermitian matrices in the large-size limit. It appears in applications as diverse as random permutations, random tilings and growth models. The distribution has proved difficult to compute numerically, particularly in the "general beta" setting that extends the classical real/complex/quaternion triad to a family parametrized by a continuous "temperature" parameter in connection with statistical mechanics. We compute the general-beta Tracy-Widom distribution by solving a linear parabolic PDE. The PDE has some challenging features such as a non-compact domain and a degenerate diffusion term; it provides an interesting test of multiple PDE solvers, in particular one based on Chebyshev technology that should be of interest to the numerical linear algebra community.

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PP4

Max-Plus Approximation of Lu Factorization

We present a new method for the a priori approximation of the order of magnitude of the entries in the LU factors of a matrix A. Our method also predicts which permutation matrices will be chosen by Gaussian elimination with partial pivoting or complete pivoting. It uses max-plus algebra and is based purely on the moduli of the entries in the matrix. This approximation can be used in the construction of incomplete LU (ILU) preconditioners as a mean to quickly determine the positions of the largest entries in the LU factors. These positions can subsequently be used as the sparsity pattern for an ILU preconditioner.

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PP4

SVDS - Practical Aspects of Bidirectional Lanczos Method

We describe a new implementation of the MATLAB `svds` function, based on [Baglama and Reichel, Augmented Implicitly Restarted Lanczos Bidiagonalization Methods, 2005]. We discuss practical aspects of the implementation: the treatment of badly conditioned matrices, the influence of numerical error in the sparse QR factorization, and the case of singular values with multiplicities.

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PP4

Global Polynomial Rootfinding in 1D, 2D, and DD

Global polynomial rootfinding is one of the most common tasks in software packages such as Chebfun and ApproxFun. For polynomials of one and two variables, the rootfinding algorithm is quite robust and practical, even when the polynomial degrees are in the thousands. However, for higher dimensional rootfinding we have shown that the two popular resultant-based methods are numerically unstable by a factor that grows exponentially with the dimension. This poster will tell the ongoing saga.

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PP4

A Class of Preconditioners Based on Low-Rank Approximation Techniques

We propose a class of approximate inverse preconditioners. The SLR preconditioner focuses on the Schur complement in any standard domain decomposition framework and tries to approximate its inverse by the inverse of the submatrix corresponding to the interface points plus a low-rank correction term. The MSLR preconditioner further exploits

the hierarchy among the interface points to improve scalability for large scale problems. Their robustness has been tested through various sparse matrices stemming from different backgrounds.

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PP4

The Shift and Invert Lanczos Algorithm for the Solution of Structural Dynamics Problems

To accurately describe the behaviour of a structure under dynamic loading, structural engineers require the smallest number ℓ of eigenvectors x_j, $j = 1, \dots, \ell$, of the symmetric definite generalized eigenvalue problem $Kx = \lambda Mx$ with stiffness matrix K and mass matrix M, that satisfy

$$\sum_{j=1}^{\ell} \phi(x_j) > 0.9, \qquad \phi(x_j) = \frac{(x_j^T Mr)^2}{r^T Mr},$$

where r is the rigid body vector. Towards this goal, we present a restarted shift-and-invert Lanczos algorithm, which improves upon existing algorithms for this problem by achieving the application-required 90% mass participation target.

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PP5

Minisymposterium: A Mathematical Investigation of Vaccination Strategies in a Heterogeneous Population to Prevent Measles Epidemics

This presentation focuses on an investigation of vaccination strategies to prevent measles epidemics. An SVIR model was created to investigate the process of how an epidemic of measles can spread within a heterogeneous population where a portion of each sub population has been vaccinated. Included in the SVIR model is a contact matrix, which represents the level of interaction between the subpopulations and within each sub-population itself. This project considers an overall population that is divided into two sub-populations. Simulations from the model are used to predict the reproductive number (a value that is used to evaluate how rapidly a disease may spread) for the total population based on differing vaccination levels within each subpopulation. Results from a variety of interaction scenarios will be presented.

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PP5

Minisymposterium: Modeling the Spread of Measles with Pockets of Low Vaccination Coverage Rates

While the national and state vaccination coverage rates of measles remain high, recent news have shown several outbreaks, which may be due to pockets of low vaccination coverage. We study this phenomenon by modeling vaccination rates in communities in Ohio. We have developed a spatial S-V-I-R (Susceptible-Vaccinated Infected-Recovered) model. Mathematical analysis and numerical simulations are conducted to investigate the outbreak occurrence with travel between low and high vaccinated communities.

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PP5

Minisymposterium: Mathematical Modeling of Dengue

Mathematics can be used to model the transmission of diseases. One method of doing so is through the use of differential equations. Populations are modeled using equations that describe the rates of change of the different parts of the population the flow in and flow out of the population. In disease modeling, the population is commonly divided into susceptible, those who can catch the disease, infectious, those who have the disease and can pass it on to others, and recovered, those who had the disease, but no longer do and cannot get it again. A system of differential equations is created that describe the rates of change of these populations over time based on parameters specific to the disease, such as how likely someone is to catch the disease after being exposed to it, and how long someone will be infectious after contracting the disease.

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PP5

Minisymposterium: Working in the City and Getting Dengue Fever: A Mathematical Model of Dengue Fever Incorporating Mobility

Dengue fever is transmitted by day-biting mosquitoes in tropical urban areas. There is currently no vaccine for dengue fever or for the fatal form of the disease, dengue hemorrhagic fever and dengue shock syndrome, so preventative measures are the only solution to slow the spread of the disease. Mathematical modeling can be used to help investigate methods of intervention. In order to model dengue fever, an SIR model can be used to describe the dynamics of the susceptible (S), infected (I) and recovered (R) humans and mosquitoes. Previous research by Lourdes Torres-Sorando and Diego J. Rodrguez incorporated the framework of an SIR model to create a visitation model for malaria. The model simulates malaria spreading between two patches, which is similar to showing how dengue fever spreads when individuals in a community leave their area to go to work in a different area. Additional analysis was conducted on an SIR dengue transmission model developed by Lourdes Esteva and Cristobal Vargas. The visitation concepts of the Torres-Sorando and Rodrguez model were then incorporated into the Esteva and Vargas model in order to show humans traveling between two areas and being infected with dengue. A preliminary system of ordinary differential equations has been generated using both of the models and future research will be conducted on the biting rate as a function of time as well as on the models fit for dengue.

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PP6

Working with Big Data in Matlab

Big data refers to working with datasets that are too big to fit into memory. We present the MATLAB `datastore` paradigm and related `mapreduce` capability, which provide a systematic way to work with such datasets in MATLAB, whether computing locally on a desktop or scaling up to Hadoop(R).

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PP6

Mixed-Integer Optimization with Matlab and Optimization Toolbox

The MATLAB environment enables building complex optimization algorithms, including chaining together existing solvers. Examples, including robust portfolio optimization built from mixed integer and nonlinear solvers in Optimization Toolbox, will be shown.

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PP6

Computational Geometry in Matlab

Functions in computational geometry have been in MATLAB for many years. Recently MATLAB added the capability to create 2D and 3D alpha shapes from a set of points. Users can subsequently perform a set of queries on the alpha shape. Several other functions such as triangulation and nearest neighbor search were optimized to give more accurate results.

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PP7

RKToolbox: A Rational Krylov Toolbox for MATLAB (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

RKToolbox consists of algorithms based on rational Krylov techniques, a gallery of examples covering a range of applications, and additional utility functions. The core of the toolbox is a flexible implementation of rational Arnoldi. Other main features include the RKFIT algorithm (may be used to find poles for rational Krylov spaces if a smaller surrogate problem is available), and the RKFUN class (allows numerical computing with rational functions). The toolbox is available on `http://rktoolbox.org/`.

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PP7

Density of States for Graph Analysis (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

Most spectral graph theory relates graph properties to extreme eigenvalues and associated eigenvectors of a graph matrix (the random walk matrix, combinatorial Laplacian, the adjacency matrix, etc). Borrowing from condensed matter physics, we connect graph properties to global eigenvalue distributions (density of states) and eigenvalue distributions weighted by node participation (local density of states). We describe efficient methods to compute spectral densities, and illustrate through analysis of several large-scale networks.

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PP7

Nonlinear Model Reduction in Computational Fluid Dynamics

Developing effective reduced-order models (ROMs) for compressible, turbulent fluid flows is a challenging problem whose solution can enable an important breakthrough: the routine use of large eddy simulation (LES)—or even direct numerical simulation (DNS)—models in time-critical applications such as aircraft design. We present a number of advances to making this goal a reality, including 1) least-squares Petrov–Galerkin projection (which exhibits superior accuracy to Galerkin projection), 2) the sample-mesh concept (which enables small-footprint ROM simulations), and 3) structure preservation (which ensures the ROM conserves mass, momentum, and energy globally).

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PP7

Discovering and Visualizing Active Subspaces (byod: Bring Your Own Data) - (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

I will show several examples of discovering low-dimensional structure in functions of several variables using active subspaces and related tools from statistics for sufficient dimension reduction.

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PP7

Information Flow in Transient Network Dynamics

The dynamical evolution of a complex system is characterized by the sharing and flow of information among the individual components. For dynamical processes such as the synchronization of networks, essentially no information can be extracted after the system settles to its (synchronization) attractor. Instead, we focus on the transient dynamics and show that the information flow computed from the transient states can effectively reveal topological properties of the underlying network dynamics.

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PP7

Erasure Coding for Fault Oblivious Linear System Solvers (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

We propose an alternate approach to dealing with system faults, which is an algorithmic analog of erasure coded storage. It applies a minimally modified algorithm on an augmented input to produce an augmented output. The execution of such an algorithm proceeds completely oblivious to faults in the system. In the event of one or more faults, the true solution is recovered using a rapid reconstruction method from the augmented output. We demonstrate this approach on the problem of solving sparse linear systems using a conjugate gradient solver. Preprint: http://arxiv.org/abs/1412.7364

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PP7

Interactive Demo of Graph Algorithms in MATLAB (Part of PP6 Minisymposterium: Mathworks)

We present an interactive demo of the graph algorithms included in MATLAB. This demo is a hands-on experience which encourages conference participants to experiment with directed and undirected graphs in MATLAB. For instance, we show live examples based on the co-authorship graph of the 2016 SIAM Annual Meeting participants. We also welcome conference participants to bring their own graphs and experiment with the latest graph algorithms included in MATLAB.

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PP7

A High-Performance Parallel Algorithm for Nonnegative Matrix Factorization (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

Non-negative matrix factorization (NMF) is the problem of determining two non-negative low rank factors $\mathbf{W}$ and $\mathbf{H}$, for the given input matrix $\mathbf{A}$, such that $\mathbf{A} \approx \mathbf{WH}$. NMF is a useful tool for many applications in different domains such as topic modeling in text mining, background separation in video analysis, and community detection in social networks. Despite its popularity in the data mining community, there is a lack of efficient distributed algorithms to solve the problem for big data sets. We propose a high-performance distributed-memory parallel algorithm that computes the factorization by iteratively solving alternating non-negative least squares (NLS) subproblems for $\mathbf{W}$ and $\mathbf{H}$. It maintains the data and factor matrices in memory (distributed across processors), uses MPI for interprocessor communication, and, in the dense case, provably minimizes communication costs (under mild assumptions). As opposed to previous implementations, our algorithm is also flexible: (1) it performs well for both dense and sparse matrices, and (2) it allows the user to choose any one of the multiple algorithms for solving the updates to low rank factors $\mathbf{W}$ and $\mathbf{H}$ within the alternating iterations. We demonstrate the scalability of our algorithm and compare it with baseline implementations, showing significant performance improvements.

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PP7

Making Machine Learning Workflows Easy (Part of PP6 Minisymposterium: Mathworks)

Applying machine learning techniques to real data presents a number of problems, including understanding the wealth of techniques available and making valid (principled) decisions about training and accuracy. We describe our experiences in producing an app (GUI) to provide a variety of techniques of varying complexity such as discriminant analysis, support vector machines, random forests, and other advanced ensemble methods including boosted decision trees. The app encourages feature selection, visualization, cross-validation, and other good practices.

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PP7

Does Your MATLAB Code Pass the Test? Tools for Testing for MATLAB Code (Part of PP6 Minisymposterium: Mathworks)

When you write code in MATLAB, how confident are you that the code does what you intend? In this poster you will learn about sets of tools (some new in the most recent release!) that you can use to test your code for correctness and performance. This poster will cover tools for novice, experienced, and master users of MATLAB.

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PP7

Iterative Regularization Tools – A Matlab Package for Large Scale Inverse Problems (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

We describe and demonstrate a new MATLAB software package that consists of state-of-the-art iterative methods to solve large scale ill-posed inverse problems. The package allows users to easily experiment with different iterative methods (including several new approaches) and regularization strategies with very little programming effort. The package includes several test problems and examples to illustrate how the iterative methods can be used on a variety of large-scale inverse problems.

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PP7

The Humility Project: Text Analysis for Characteristic Linguistic Patterns

This interdisciplinary text analysis research project aims to develop a classifier for documents based on the presence or absence of humility. In our method of Latent Semantic Analysis, we utilize Nonnegative Matrix Factorization (NMF) as a low-rank matrix approximation. We designed a novel global weight that performed well for exploratory clustering to learn about different types of humility. The IDF global weight performed better for classification through cross-validation (66% accuracy).

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PP7

3D Visualization of Growth Pattern of Artemisia Tridentata (Sagebrush)

Plants of Artemesia tridentata (sagebrush) are dominant in the American southwest. Many species of Artemesia tridentate show extensive eccentric growth, which probably limits its ability to grow tall. Eccentric growth occurs because the vascular cambien dies and does not continue to produce secondary xylem in stems. The purpose of this study is to create an accurate pictorial representation of xilary ring growth of an eccentric stem of Artemesia tridentata using computer visualization. Three xylary rings were visualized using MATLAB in a three dimensional representation which allowed the discontinuation of the rings from segment to segment to be viewed. The eccentric growth is quite localized and the growth rings in one location seemingly have little effect on the growth on nearby locations.

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PP7

Spectra of Short Pulse Solutions of the Cubic-Quintic Complex Ginzburg Landau Equation Near Zero Dispersion

The cubic-quintic complex Ginzburg Landau (CQCGL) equation provides a simple model for studying the short pulses generated by mode-locked fiber lasers. We numerically compute stationary solutions of the CQCGL equation near zero dispersion and determine both their stability and the spectrum of the linearized operator. We show that as the chromatic dispersion parameter varies continuously from positive to negative, there is a continuous family of stable stationary solutions. However, the number of discrete eigenvalues and the configuration of the discrete and continuous spectrum in the complex plane undergoes a qualitative change as the sign of the dispersion changes from the anomalous regime to the normal regime.

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PP7

How You Can Improve the Scalability of your PDE Solver by Using Swept Domain Decomposition

Future engineers will design economic and capable aerospace vehicles and engines using high fidelity simulations. To enable this future, such simulations must run significantly faster than today. What prevents simulations from running faster is no longer just the amount of computation power. Communication latency between processors is becoming a main barrier for simulations based on partial differential equations. This animation will illustrate how we can decompose space and time in non-conventional fashions, to effectively break the latency barrier, while using many existing numerical schemes.

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PP7

Clustering of Omics Data in Biological Systems

Big data including DNA sequence, RNA, and protein data rises in many biological systems. Quantitative and qualitative modeling of these systems needs precise assessment and deep understanding of system functioning. In modern metagenomics, there are many potentially interacting objects (species, cell populations, molecules, etc.) of interest, which may need to be modeled via dynamics systems and lead to an explosion in the number of parameters. We propose an innovative model-based clustering technique to infer from time series or time course data. The estimation procedure is an iterative algorithm and this procedure is assessed to be feasible via a simulation study. Also many variables or features per sample (patient, etc.) are measured, for example, levels of thousands of mRNA and proteins in hundreds of samples are collected, and such high dimensionality make visualization and interpretation of samples difficult and limit exploration of data. We develop a new clustering technique which is equivalent to finding dimensionality of data via principal component analysis (PCA), removing outliers and implementing clustering to groups the principal component loadings on projected space. Computational study show that our technique produce the best results. This technique can also help select the best metric for hierarchical clustering in the data set.

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PP7

A Randomized Tensor-SVD Algorithm with Applications in Image Processing (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

The tensor Singular Value Decomposition (t-SVD) proposed by Kilmer and Martin [2011] has been applied successfully in many fields, such as computed tomography, facial recognition, and video completion. In this talk, I will present a probabilistic method that can produce a factorization with similar properties to the t-SVD, but is stable and more computationally efficient on very large datasets. This method is an extension of a well-known randomized matrix method. I will present the details of the algorithm, theoretical results, and provide experimental results for two specific applications.

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PP7

Multifrontal Sparse Matrix Algorithms in Julia (Part of PP4 Minisymposterium: Algorithms and Software in Numerical Linear Algebra)

We introduce Multifrontal.jl, a Julia software for solving sparse matrix systems using the multifrontal method. In contrast to the current black-box C and Fortran implementations, our high-performance code is easy to read and understand. The package contains a serial and shared-memory parallel implementation of multifrontal Cholesky, LU, and QR factorization. Taking advantages of Julia's type system and the GNU MPFR Library, Multifrontal.jl also supports arbitrary precision arithmetic.

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LS16 Abstracts

Art courtesy of Bourouiba, Gourley, Liu and Wu, SIAP 71-2

IC0

Cowan Cancelled

Abstract not available at time of publication.

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IC1

Beating in Fluid: Hearts and Cilia by the Immersed Boundary Method

The immersed boundary (IB) method treats immersed elastic bodies or boundaries as if they were a part of the fluid in which additional forces are applied. In the context of the beating heart, this makes possible the simultaneous simulation of the thin, flexible heart valve leaflets and the thick, muscular heart walls, along with the blood flow in the cardiac chambers; and it turns out that the IB methodology is also well suited to the simultaneous numerical solution of the bidomain equations of cardiac electrophysiology. The problem of beating cilia is one of synchronization. How do the hundreds of dynein motors distributed within a given cilium coordinate to achieve the ciliary beat, and then at a higher level, how do the multiple cilia of an array coordinate their beating to move fluid? We introduce a phenomenological model in which each dynein motor obeys a simple dynamical law and in which both types of coordination emerge spontaneously. This talk describes joint work with Boyce Griffith, Jihun Han, Alexander Kaiser, and David McQueen.

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IC2

Mathematical Models for Cell Polarization and Gradient Sensing

Directed or polarized growth and the detection of chemical gradients are two fundamental cellular processes. Here we combine mathematical modeling with various experimental approaches to investigate the molecular mechanisms that underline both processes during the mating response of Saccharomyces cerevisiae (budding yeast). Our analysis reveals a novel method for gradient sensing and insight into the biochemical mechanisms that ensure the establishment of a unique polarity site.

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IC3

Qualitative Features of Transient Responses A Case Study: Scale-Invariance

This talk will review the biological phenomenon, and formulate a theoretical framework leading to a general theorem characterizing scale invariant behavior by equivariant actions on sets of vector fields that satisfy appropriate Lie-algebraic nondegeneracy conditions. The theorem allows one to make experimentally testable predictions, and the presentation will discuss the validation of these predictions using genetically engineered bacteria and microfluidic devices, as well their use as a "dynamical phenotype" for model invalidation. The talk will also include some speculative remarks about the role of the shape of transient responses in immune system self/other recognition and in cancer immunotherapy.

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IC4

Rational Design of Tissue Engineered Heart Valves

Valve replacement with mechanical or bioprosthetic prostheses is the most common intervention for valvular disease, with almost 300.000 annual replacements worldwide. However, in particular in patients younger than 18 years freedom from reoperation is only 58-68% at 15 years. Tissue engineering of living heart valves seeks to overcome these limitations. One of the most critical problems in heart valve tissue engineering is the progressive development of valvular insufficiency. In an effort to resolve this challenge, a computational model was developed to predict the in vivo remodeling process in tissue engineered heart valves subjected to dynamic pulmonary and aortic pressure conditions, and to assess the risk of valvular insufficiency.

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IC5

The Turbulent Life of Plankton

Plankton in oceans and lakes is often exposed to turbulence, yet only recently have quantitative models begun to emerge to describe the effects of turbulence on the physiology and behavior of planktonic cells. I will illustrate the unexpected effects of turbulence on plankton by focusing on motile phytoplankton cells - photosynthetic organisms that form the base of most aquatic food webs - through both millifluidic experiments and mathematical models. I will propose that phytoplankton, despite their small size, know more fluid mechanics than we give them credit for, and will highlight how the turbulent life of plankton presents a plethora of opportunities for both the experimenter and the mathematical modeler, who together can help advance our understanding of these pivotal players in some of earth's most vital ecosystems.

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IC6

Follow the Yellow Brick Road: Mathematical Insights into Virus Structure enable Discovery in Virus Assembly and Evolution

Viruses are remarkable examples of order at the nanoscale. The vast majority of viruses package their genomes into protective protein containers that are organised according to icosahedral surface lattices. This has far reaching consequences for many stages of the viral life cycle and the infection process overall. In this talk, I will demonstrate how we have used mathematical approaches, developed in my group for the characterisation of virus architecture, to gain unprecedented insights into how viruses form and evolve.

In a recent commentary in the Journal of Molecular Biology (see PubMedID 26707196) Peter Prevelige has described this approach as "following the yellow brick road". In this talk, I will invite you on a journey along the yellow brick road. I will introduce the mathematical tools underpinning our approach and demonstrate how they have contributed, in collaboration with experimentalists, to a paradigm shift in our understanding of virus assembly. I will moreover describe how these results open up a new perspective on viral evolution and anti-viral therapy.

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IC7

Impact of Quantitative and Systems Pharmacology in Drug Discovery and Development: It is all about the Question

The pharmaceutical industry must reduce costs while delivering innovative medicines with improved benefits for patients. With increasing computational capability, scientists can leverage quantitative tools to answer critical questions that influence the discovery and development of important new medications. These new approaches and tools have led to the expansion of a specialized field, quantitative and systems pharmacology (QSP, sometimes called modeling and simulation). Quantitative and Systems Pharmacology is an integrative science incorporating relationships between diseases, drug characteristics, and individual variability to leverage existing knowledge and guide future research. QSP helps define the questions and assumptions and highlights knowledge gaps. Through this approach it is possible to estimate drug efficacy, understand safety, plan experiments, and inform discovery/development strategies. Examples that highlight the ability to answer such questions as 1) should this molecule be developed as a drug, 2) what is the right dose to balance efficacy and safety, and 3) does this new drug increase bone strength will be presented. The ultimate goal is not a mathematical model but rather the ability to gain insight to optimize new medications for patients.

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IC8

Parkinsonian Oscillations: A Computational View

Parkinsons disease is a debilitating condition causing highly disruptive motor complications. It also provides a range of opportunities for the application of computational and mathematical methods to provide a better understanding of the mechanisms involved and to optimize therapeutic approaches. In particular, there are questions to address concerning the origins of parkinsonian changes in neural synchrony, oscillations, and correlations, the translation of these changes into motor pathologies, the effects of therapeutic interventions involving brain stimulation that somehow alter this activity, and the derivation of control strategies. I will discuss my perspective on some of these challenges and highlight some examples of approaches to tackling them.

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SP1

AWM-SIAM Sonia Kovalevsky Lecture - Biofluids of Reproduction: Oscillators, Viscoelastic Networks and Sticky Situations

From fertilization to birth, successful mammalian reproduction relies on interactions of elastic structures with a fluid environment. Sperm flagella must move through cervical mucus to the uterus and into the oviduct, where fertilization occurs. In fact, some sperm may adhere to oviductal epithelia, and must change their pattern of oscillation to escape. In addition, coordinated beating of oviductal cilia also drives the flow. Sperm-egg penetration, transport of the fertilized ovum from the oviduct to its implantation in the uterus and, indeed, birth itself are rich examples of elasto-hydrodynamic coupling. We will discuss successes and challenges in the mathematical and computational modeling of the biofluids of reproduction. In addition, we will present reduced models that evoke intriguing questions in fundamental fluid dynamics.

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SP2

The John Von Neumann Lecture: Satisfiability and Combinatorics

The Satisfiability Problem, which asks whether or not a given Boolean formula can be satisfied for some values of its variables, has long been thought to be computationally hopeless. Indeed, SAT is the well-known "Poster Child" for NP-complete problems. But algorithmic breakthroughs have made it possible for many important special cases of the problem to be solved efficiently. Industrial-strength "SAT solvers" have become a billion-dollar industry, and they play a vital part in the design of contemporary computers. The speaker will explain how the new SAT technology also helps us to solve a wide variety of problems that belong to combinatorial mathematics.

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SP3

W.T. and Idalia Reid Prize in Mathematics: Data and the Computational Modeling of Complex Systems

In mathematical modeling one typically progresses from observations of the world (and some serious thinking!) to equations for a model, and then to the analysis of the model to make predictions. Good mathematical models give good predictions (and inaccurate ones do not) - but the computational tools for analyzing them are the same: algorithms that are typically based on closed form equations. While the skeleton of the process remains the same, today we witness the development of mathematical techniques that operate directly on observations -data-, and "circumvent" the serious thinking that goes into selecting variables and parameters and writing equations. The process then may appear to the user a little like making predictions by "looking into a crystal ball". Yet the "serious thinking" is still there and uses the same -and some new- mathematics: it goes into building algorithms that "jump directly" from data to the analysis of the model (which is never available in closed form) so as to make predictions. I will present a couple of efforts that illustrate this new path from data to predictions. It really is the same old path, but it is travelled by new means.

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SP4

I. E. Block Community Lecture: Toy Models

Would you like to come see some toys? 'Toys' here have a special sense: objects of daily life which you can find or make in minutes, yet which, if played with imaginatively, reveal surprises that keep scientists puzzling for a while. We will see table-top demos of many such toys and visit some of the science that they open up. The common theme is singularity.

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JP1

Spatio-Temporal Dynamics of Childhood Infectious Disease: Predictability and the Impact of Vaccination

Violent epidemics of childhood infections such as measles provide a particularly clear illustration of oscillatory 'predator-prey' dynamics. We discuss limits on the predictability of these systems, both in the era before vaccination and at present, where vaccine hesitancy limits the effectiveness of vaccination programs in many countries. We also discuss the impact of viral evolution on predictability and the design of vaccination programs, with particular reference to influenza and rotavirus.

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CP1

When Can Michealis-Menten or Hill Functions Lead Accurate Stochastic Simulations?

The non-elementary reaction functions (e.g. Michaelis-Menten or Hill functions) are frequently used as propensities of Gillespie algorithm. Despite their popularity, it remains unclear when such stochastic reductions are valid. Here, we first identify the validity condition for using non-elementary reaction functions for the stochastic simulations. This provides a simple and computationally inexpensive way to test the accuracy of reduced stochastic model.

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CP1

Systems Analysis of Nfκb Signaling System Reveals Signaling Nodes and Their Robust Features Controlling Transcriptional Outcome

The NFκB signaling system is important during healthy and pathological responses to inflammatory stimuli. Although many molecular components of this system are known, their connectivity and quantitative influences on downstream transcriptional responses are less well defined. Previous work from our lab identified the importance of signal fold-change in predicting transcriptional outcome. Experiments and detailed mathematical modeling done in this work indicate that the sensitivity of fold-change is modified by additional regulatory loops downstream.

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CP1

Origin of Balanced Growth, Homeostasis and Bacterial Growth Laws in Growing-Dividing Models of Cells

We have considered a new class of well stirred chemical dynamical systems that grow and divide like cells under the control of an internal 'division variable'. We have formulated the conditions under which such systems can robustly reach a balanced growth-division steady-state wherein the doubling of thousands of chemical species are coordinated to happen at the same time and hence enabling self-replication. This robust mechanism explains the origin of homeostasis and stable distributions of size, composition, inter-division time etc. in the steady-state. For a simple protocell model, we have derived the explicit expressions for the growth rate and chemical composition at the steady-state in terms of the cellular and medium parameters. We show why chemicals exhibit exponential growth with time in spite of their complex nonlinear dynamics and discuss cases when it's not. We also obtain analytical derivation of 'growth laws', namely, the dependence of ribosomal protein fraction on medium quality and antibiotics by assuming an additional regulatory mechanism that regulates the production of the ribosomal and non-ribosomal proteins to optimise fitness. Our work also has implications for the Origin of Life problem, suggesting that a certain class of protocells would have been extremely robust. We also suggest a simple explanation for the currently observed phenomenon of E. Coli cells displaying the constant 'adder' property in the steady state.

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CP1

Delayed Stochastic Simulation Modelling of Stalled Transcription in Prokaryotes

Bratsun et al. (2005) proposed an algorithm to study stochastic fluctuations prevailing due to low copy number and time delays resulting from lengthy reaction sequences. We are currently studying a simple delay stochastic model for RNA transcription during stalled transcription. Roussel and Zhu (2006) showed that delay stochastic simulation algorithm shows deviations from detailed stochastic simulations at high traffic densities and we attempt to correct these defects without resorting to fully detailed simulations of transcription.

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CP1

Solving the Chemical Master Equation by an Adaptive Finite State Projection Method

The chemical master equation (CME) provides a useful tool to identify models of stochastic gene networks. We present an algorithm for approximating the solution of the CME by a novel combination of stochastic simulation, finite state projection and Krylov subspace techniques. Alternative error estimates are introduced to reduce the requirement on projection size in larger problems. We also discuss the potential of a parallel CME solver based on our method.

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CP2

Leveraging Sparsity to Detect Structural Variants in Genomic Data

Structural variants (SVs), rearrangements of the genome, occur through deletions, duplications, insertions, and inversions. These genomic imbalances contribute to genetic variation, but have been associated with certain genetic diseases. We implement a maximum likelihood approach using sparsity of SVs to detect variants in sequencing data. To model inheritance of SVs, we incorporate parental constraints in our optimization in reconstructing child signal observations. We present numerical results of simulated and real sequencing data in our validation.

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CP2

Immune Epitope Database and Analysis Resource (iedb)

The rapid growth in biomedical data available in publications presents researchers with a formidable challenge. The IEDB offers easy searching of experimental antibody and T cell epitope data studied in humans, non-human primates, and other animal species. Epitopes involved in infectious disease, allergy, autoimmunity, and transplant are included. We describe the process employed to populate the database and the means for accessing the data. We also describe the IEDB capabilities for predicting and analyzing epitopes.

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CP2

Mechanistic Modeling of Subpopulation Structures for Multivariate Single-Cell Data

The elucidation of sources of heterogeneity is crucial to fully understand biological processes. We propose a method that combines mixture modeling with mechanistic modeling of higher-order moments of the data. This method detects differences between subpopulations and experimental conditions using e.g. L1-regularization, and exploits cell-to-cell variability within a subpopulations. Assessing our method for artifical and real data of NGF-induced Erk signaling suggests that it is a promising tool for the analysis of single-cell data.

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CP2

Interlaboratory Comparison and Reproducibility Analysis of Nuclear Magnetic Resonance Spectroscopy Using Cluster Analysis

Data quality in metabolomics may be assessed directly using raw spectra before time-consuming identification and quantification. This paper demonstrates using raw NMR spectra to conduct detailed inter-laboratory comparison and composition analysis. Spectra of biological tissue samples, obtained by several laboratories, are compared with cluster analysis using a variety of distance and entropy metrics. We evaluate where individual measurements fall within their clusters to develop an estimate of each laboratorys performance.

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CP2

ddPCR and qPCR Accuracy Comparison Using Probability Theory and Computation

Digital Droplet PCR (ddPCR) appears to offer increased accuracy in HIV copy measurements when compared to quantitative PCR (qPCR). We have developed a novel recursive formulation of the exact likelihood function for ddPCR, for use in Bayesian model fitting from patient data. This formulation is also used to to compare the theoretical limits of the accuracy of ddPCR and qPCR. It is shown that ddPCR provides significantly more information for system identification compared to qPCR.

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CP3

Parameter Estimation for Gene Regulatory Network Modeling

We investigate the dynamics of a gene regulatory network that controls the cold-shock response in budding yeast, Saccharomyces cerevisiae. Using microarray data from wild type and knock-out strains, we infer the parameters of a dynamical systems model that balances production and degradation of RNA. While the network connections are determined from other published sources, the strength of the regulatory relationship and the sign (activation or repression) are inferred using our penalized least square approach.

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CP3

Understanding the Role of Mitochondria Distribution in Calcium-Induced Exocytosis in Bovine Chromaffin Cells

Adrenomedullary chromaffin cells are widely used as a valuable model to study calcium-induced exocytosis of dense vesicles. Functional studies demonstrated the important role of organelles in shaping calcium signals in this cell type. Therefore the study of mitochondria distribution in relation with exocytotic sites is relevant to understand the nature of such modulation. In this talk we discuss the spatial distribution of mitochondria in bovine chromaffin cells in culture inferred from experimental observations and use a theoretical model for understanding the role played by these organelles in the fine tuning of calcium signals and the modulation of secretion.

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CP3

Improved Ergodicity and Mixing Estimators for Single Particle Tracking

We propose the improved ergodicity and mixing estimators to identify nonergodic dynamics from a single particle trajectory. The estimators are first investigated for several models of anomalous diffusion, including nonergodic CTRWs. The estimators are then applied to two sets of experimental trajectories, revealing ergodic and nonergodic behaviors separately for each trajectory and providing thus a more flexible analysis of single-particle tracking experiments in microbiology.

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CP3

A Stability Analysis of the Biological Networks, Transcriptional Network, Neural Circuit and Ecosystem

The three types of biological networks, transcriptional network, neural circuit and ecosystem, were described by similar mathematical models, and common dynamics are suggested. We studied the two-body models of the networks and report here: vector fields by the network models are very similar; analyses on the trace-determinant plane from the Jacobian matrix suggested self-interactions are the primary factor for stable coexistence of the network components; gradients of mutual interactions and self-degradations affect the stable coexistence.

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CP3

Volume-Excluding Diffusion Models at Varying Spatial Scales

Diffusion is integral to many biological processes, and lattice-based position-jump models are a popular choice for interrogating them. In this talk, I outline both coarse- and fine-grained lattice-based models for diffusion, and demonstrate the connection between the two. I also describe hybrid models combining coarse- and fine-grained models. These hybrid models take less time to simulate than exclusively fine-grained models, but provide increased accuracy compared to coarse-grained models where needed.

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CP4

An Integrative Modeling Framework for in Vivo Tissue Regeneration

In vivo human tissue regeneration is one of the greatest challenges in medicine. Despite of a great deal of experimental findings, complexity hinders theoretical framework developments which impose expensive experimentation based in animal models. Considering, that in biological tissues complexity comes from the close dynamical coupling between cell populations and physical fields, a software framework based in FEM, Lattice Boltzmann and Cellular Automata is proposed and presented for the integrative mathematical modeling of biological tissues.

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CP4

Scalable Simulation of Systems of PDEs for Modeling Tumor Growth

There are existing sophisticated mathematical models designed to model tumor growth with partial differential equations (PDEs); however, finding solutions is computationally expensive so researches have to lower resolution, simplify models, or run fewer simulations with representative sets of parameters, etc. Thus, results are less accurate, less timely, or not tailored to individual patients. We hypothesize that, a component-wise time-stepping method can be used so that greater accuracy, efficiency and scalability can be achieved.

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CP4

A Mathematical Model to Elucidate Brain Tumor Abrogation by Immunotherapy with T11 Target Structure

T11 Target structure (T11TS), a membrane glycoprotein isolated from sheep erythrocytes, reverses the immune suppressed state of brain tumor induced animals by boosting the functional status of the immune cells. This study aims at aiding in the design of more efficacious brain tumor therapies with T11 target structure. We develop a mathematical model for malignant gliomas or brain tumor and the immune system interactions, by introducing the role of immunotherapeutic agent/drug T11TS. The model encompasses considerations of the interactive dynamics of malignant glioma cells, macrophages, cytotoxic T- lymphocytes (activated CD8+ T - cells), immune-suppressive factor TGF-β , immune-stimulatory factor IFN-γ and the T11TS. We performed sensitivity analysis in order to determine which of the state variables are more sensitive to the given system parameters. The results of the proposed mathematical model are compared with experimental data procured by our collaborator Prof. Dr. Swapna Chaudhuri, Immunology Lab, Department of Hematology, School of Tropical Medicine, Kolkata, India. Computer simulations were used for model verification and validation, which underscore the importance of T11 target structure in brain tumor therapy.

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CP4

Identifiability of Ode Models of Tumor Growth.

ODE models for understanding and predicting basic biology, disease, and therapy in cancer research often contain many parameters. This raises the problem of *identifiability*, a prerequisite for a well-posed parameter estimation, to provide reliable and accurate parameter estimates from experimental data. A unified viewpoint and the joint use of structural and practical identifiability techniques are proposed. The relevant results are to disentangle the various causes of nonidentifiability, to provide in analytic terms guidelines to simplify nonidentifiable models or enrich experiments. Identifiability of recent models describing tumor growth and cancer individualized treatments illustrates the results.

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CP5

Mathematical Modeling and Experimental Validation of Cell Cycle and Circadian Clock Coupling in Adult Stem Cell Cultures

Circadian (24 h) clock gates cells in 3D murine intestinal organoids (enteroids) with heterogeneous individual cell cycle times to produce 12-h population cell division rhythm. Remarkably, we observe reduced amplitude circadian oscillations in these cells, indicating that an intercellular signal mediates circadian clock-dependent synchronized cell cycles. Stochastic mathematical model predicted and we experimentally validated that Paneth cell-secreted Wnt is the key intercellular coupling component that links the circadian clock and the cell cycle in enteroids.

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CP5

Model of Bacterial Chemotaxis and its Simulation

Bacterial chemotaxis is the movement of motile bacteria in the direction of higher attractant concentrations and away from repellents. In oxytaxis, cells swim towards a region with favorable oxygen concentration, and they consume oxygen. Finding optimal concentration of oxygen is important for cell metabolism and growth. The chemotactic mechanism leads to formation of a band where the density of bacteria is much higher than outside the band.

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CP5

A Deep-Learning Method for Protein-Protein Interface Residue Pair Prediction

Protein-protein interactions are important in many biological processes. The information of their interaction interfaces plays a key role in the accurate prediction of protein complex. Recently, we have studied the interface residue and residue pair predictions, which helped to predict the interface pair. Firstly, we characterized the surface residues of protein monomer by five simple geometric descriptors and employed them to discriminate the interface residues from the non-interface residues. It is found that the interior contact area of the surface residue outperforms other single features. Secondly, in order to investigate the effects of all kinds of combinations of the five features, we used backward propagated neural network to train models in the train set and selected the optimal network according to the performances in the validation set, then tested its performance in the test set and compared with other three methods. Our method, nonlinear combination of EC and IC, has a prediction accuracy of 88%, much better than other methods. In order to accurately predict the interface residue pair, the surface residues were characterized by nine features (five geometric and four physicochemical), the effects of all kinds of combinations of the nine features are tested. Interface residue pair prediction does not take the whole interface into account, so we use the sum of interface residue pairs to evaluate the interface pair.

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CP5

Structured Cell Population Models with Internal Cell Cycle

J.J. Tyson, B. Novák and others developed several models for the cell cycle of budding yeast, fission yeast and other organisms. A feature of such models is the funnel effect, by which the internal structure of the cell in the later phases of its cycle (shortly before division) is nearly independent from its structure in the earlier phases of the cycle. We study the behaviour of the cells at the population level by incorporating a model of this type in a structured cell population ODE model in a chemostat with constant influx of nutrient. We investigate the behaviour of the population of cells and in particular the equilibrium states, i.e. constant distributions of the masses of cells born per unit of time. Numerically, we obtain the equilibria as fixed points of a map, namely the output of a large collection of integrations over age for cells born with a given birth mass, combined with a count of the consumption of nutrient during the age integrations. The meshless discretization of the birth mass space is adapted after each age integration cyclus. We study the equilibria numerically under parameter variation. Natural parameters are the concentration of nutrient in the feeding bottle and the influx rate of the nutrient, which is also the death rate of the cells. We numerically compare the merits of three different strategies for the numerical continuation of equilibria of the cell population model, including a variant of pseudo-arclength continuation.

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CP5

Computational Modeling of Calcium Transient Response in Urinary Bladder Smooth Muscle Cell

Urinary incontinence (UI) is involuntary urination, which has a large impact on quality of life. Detrusor smooth muscle (DSM) instability is a major cause of UI. We established a mathematical platform of sufficient biophysical detail to quantitatively simulate calcium transient based on ionic currents in DSM cell. This model provides an elementary tool to investigate the physiological calcium dynamics underlying the contractions in DSM cells, which in turn can shed light in genesis of UI.

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CP5

Stability Analysis of Signal Peptide Mutants

Recombinant thioredoxin with N-terminus malE and pelB signal sequences were studied with respect to their stability against proteolytic digestion and different guanidine concentrations via thermal shift assay. Results were compared with wild type thioredoxin without a signal sequence and its signal peptide mutants. Proteolysis of recombinant proteins results in rapid digestion of the signal peptide, suggesting that it is accessible to protease and has only transient interactions with the rest of the protein in the native state. TSA in both the cases suggests reduced stability for recombinant proteins. These studies show that besides acting as address labels, signal sequences can modulate protein stability and aggregation in a sequence dependent manner.

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CP6

Predicting the Number of Multiple Chronic Conditions in Older Adults in Us-Mexico Border Using Rapidminer

Multimorbidity prediction model was not found in literature, neither the common patterns. The varying numbers and patterns of co-morbidity create a challenge for healthcare providers; it affects the delivery of an efficient treatment and care coordination plans. We used Rapidminer data mining tool to predict the number chronic conditions and identify the most common pattern of multimorbidity in Arezona using SID HCUP Data set. Classification algorithms gave the best results among other algorithms we tried.

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CP6

Modeling the Impact of Screening and Partner Notification on Chlamydia Intervention in New Orleans

We created and analyzed an individual network-based model for the spread of the sexually transmitted infection, chlamydia trachomatis, in New Orleans. Chlamydia is the most common sexually transmitted infection in the United States with over 1.8 million cases each year. This includes approximately 12% of African American women and 8% of men between 15-25 years old currently infected in New Orleans. Chlamydia is the major cause of infertility, pelvic inflammatory diseases and ectopic pregnancy among women and been associated with increased HIV acquisition. We created a weighted bipartite sexual partnership network for men and women that captures biased heterosexual mixing between the risk groups. We then use a stochastic agent-based Markovian epidemic model to quantify the effectiveness of mitigation methods, such as screening and partner notification, in controlling the epidemic. Our simulations were used to optimize a mitigation program based on partner notification and screening both men and women. The model verified the existence of a threshhold value for stopping the epidemic based on the fraction of an infected persons partners who are tested, and treated, for infection. We are collaborating with the Tulane School of Public Health and Tropical Medicine to use this model in helping public health officials implement effective policies in allocating resources to control the current chlamydia epidemic in New Orleans.

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CP6

Investigate the Drivers for Non-elective Admissions Among Patients in Sheffield

Non-elective admission are becoming the dominant factor in primary care and the main routes into hospital admission, as a result, there is pressure on hospitals to improve capacity (Pencheon 2015). Using a mixed methodology, comparison of multiple statistical methodology, revealed the drivers of non-elective admission in hospital.

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CP6

Development of An Expert System for Improving Post-Accident Monitoring Protocols in Nuclear Industry

In the nuclear industry, individual bioassay monitoring is performed for workers potentially exposed to radioactive contamination in order to guarantee the respect of radiation dose limits. Dosimetric evaluation software using a probabilistic tool to account for uncertainties on exposure conditions and bioassay measurements has been developed. Herein, we aim to build a decision support expert system in order to determine the best bioassay monitoring program through a utility function conditioned on dose level and uncertainty.

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CP6

A Quantitative Analysis of Statistical Power Identifies Limitations in Exploratory Studies of Obesity Endpoints in Mice

The ability to design well-powered animal studies is key to identifying and effectively testing potential drug targets. In this work we embed a previously validated mathematical model of mouse energy metabolism within a two-stage mixed effects statistical framework to capture individual mouse and endpoint variability within and between mice/endpoints. After fitting to existing data, we use the calibrated model to illustrate how different sources of endpoint variability can affect study design and conclusions.

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CP7

Fluctuating Hydrodynamic Methods for Manifolds: Protein Dynamics in Curved Lipid Bilayer Membranes

We present theory for protein diffusion and active transport within curved lipid bilayer membranes. Our theory takes into account the hydrodynamics within the two bilayer leaflets, intermonolayer slip between the leaflets, and coupling with the surrounding bulk solvent fluid. In 1975, Saffman and Delbruck introduced a hydrodynamic theory for infinite flat sheets that is still a widely used theory for the diffusivity of membrane proteins. We show for a finite curved membrane sheet that geometric and topological effects can significantly augment the protein diffusivity and hydrodynamic coupling. We present results showing how these effects contribute to the individual and collective motions of protein inclusions in spherical vesicles. We also present general fluctuating hydrodynamic methods for manifolds that can be used for general investigations of many-body systems involving diffusion and hydrodynamic transport within thin fluid interfaces having curved geometries.

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CP7

Chiari I Malformation Results in Transitional Like Hydrodynamics of the Cerebrospinal Fluid Near Cranio-Vertebral Junction - A Computational Study

Chiari malformation type I is a disorder characterized by the herniation of cerebellar tonsils into the spinal canal through the foramen magnum resulting in obstruction to cerebrospinal fluid (CSF) outflow. With direct numerical simulations consisting of up to 2 billion cells, conducted on 50000 cores of a supercomputer, we found high velocity fluctuations in the CSF near cranio-vertebral junction in patient specific models of patients with Chiari I while the flow remained laminar in the control subject.

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CP7

Numerical Aspects of Optimal Control for Water Treatment Problem

Analysis of the environmental impact of waste water discharges into aquatic media takes a great importance in the last years. The problem considered here is in the field water-quality improvement by varying the systems, such as flow regulation by means of reservoirs. The creterion functional to be minimized penalizes deviation of phaecal coliforms distribution from standard value. We adress exact controllability problems for a parabolic equation (evolution of pollutant concentration) associated with Dirac measures. Hybrid numerical methods combining particle method and finite difference method is presented. Symmetric TVD scheme for the shallow water equations, in general coordinates, is used. The technique is an hybrid method that uses the second order flux in smooth regions but involves some limiting based on the gradient of the solutions so that near discontinuities it reduces to the monotone upwind method. A particle method is proposed to handle the parabolic equation. The difficulty is then to deal with a diffusion term. We analyze an approach based on a purely deterministic method. The approximation of the diffusion operator is based on the introduction of boundary integral equation formulation. The gradient of the cost function is evaluated by adjoint techniques and the quasi-Newton as an iterative solution of the discrete control problem is choosen.

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CP7

Pulsatile Jeffrey Fluid Flow of Blood in Stenotic Arteries

In this paper, we discussed the two layered model of pulsatile blood flow in stenotic arteries. The blood flow in narrow arteries treated as two fluid model. In core region it is treated as Jeffrey fluid and in peripheral region as plasma layer, assuming Newtonian and non-Newtonian respectively. An analytic solution has been obtained of pulsatile flow of blood for various flow quantities like velocity, volume flow rate, volume flow rate, wall shear stress and flow resistance etc. The effect of various parameters like Strouhal number, Jeffrey fluid parameter, height of the stenosis etc. discussed on various flow quantities. Graphical analysis has been discussed. Keywords: Two-fluid model, Jeffery fluid, Non-Newtonian fluid, Strouhal number, pulsatile flow, Flow resistance Stenotic Arteries

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CP8

Dynamic MaxEnt Method for the Estimation of Quantitative Trait Evolution

Selection, mutation and random drift affect the dynamics of allele frequencies and consequently of quantitative traits. While the macroscopic dynamics of quantitative traits can be measured, the underlying allele frequencies are typically unobserved. Can we understand how the macroscopic observables evolve without following these microscopic processes? We approximate the allele frequency distribution, described be the Fokker-Planck equation, by its stationary form, which maximises entropy. This quasi-stationary approximation extends the current theory to the more realistic case of weak mutation.

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CP8

Permanence and Chaos in Dynamical Systems

For most ecological systems, the question of survival is tantamount. To that extent, I have been investigating whether certain chaotic three-dimensional Lotka-Volterra models are also permanent. Permanence in simple terms means the species population remain at levels safely above extinction. The goal is to show that chaos in biological systems may be beneficial to the species involved.

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CP8

The Evolution of Lossy Compression

In complex environments, there are costs to both ignorance and perception. An organism needs to track fitness-relevant information about its world, but the more informa-

tion it tracks, the more resources it must devote to memory and processing. As a first step towards an understanding of this tradeoff, we use rate-distortion theory to study large, unstructured environments with fixed, randomly-drawn penalties for stimuli confusion ("distortions'). Surprisingly, we find that two different environments will have nearly identical rate-distortion functions (but very different codebooks) when distortions are drawn from the same distribution. This suggests that the number of necessary sensory neurons, but not the specific neuronal wiring, might depend only on environmental statistics, rather than on the specifics of the environment. We further identify two distinct regimes for organisms in these structured environments: a high-fidelity regime where perceptual costs grow linearly with environmental complexity, and a low-fidelity regime where perceptual costs are, remarkably, independent of the number of environmental states. This suggests that in dynamic environments of rapidly-increasing complexity, well-adapted organisms will find themselves able to make, just barely, the most subtle distinctions in their environment.

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CP8

Cooperative Aging: The Evolutionary Dynamics Balancing Longevity and Evolvability

Cooperation is typically associated with traits or behaviors that benefit the population as a whole, but are costly to the individual. We propose that, when the environment is rapidly changing, senescence (age-related deterioration) can act as a form of cooperation. According to numerical simulations of an agent-based model, while long-lived individuals can outcompete their short lived peers, populations composed of long-lived individuals are more likely to go extinct during periods of rapid environmental change. Moreover, as in many situations where cooperative behavior arises, senescence can be stabilized in an island model.

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CP9

Predicting Opiate-Induced HIV Risk Increase

Use of opiates such as morphine and heroine upregulate a CD4+ T-cell coreceptor associated with cell infection with HIV. This upregulation likely increases the risk of HIV infection if viral exposure occurs concurrently with opiate use. We present a stochastic HIV infection model to quantify the increase in HIV risk in the presence of morphine that depends on morphine pharmacokinetics. We then discuss sensitivity of risk to HIV viral inoculum size and morphine dosage.

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CP9

Quantifying the Effect of Trypsin on Influenza Infections

Trypsin is an enzyme used to facilitate in vitro influenza infections. Trypsin cleaves the viral surface protein hemagglutinin, allowing it to fuse with the cell membrane and enter the cell. We use data from in vitro influenza infections in the presence and absence of trypsin to parameterize a within-host mathematical model of influenza infection. This allows us to quantify the dynamical changes caused by the presence of trypsin.

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CP9

Mathematical Models of HIV and HPV Coinfection in the Oral Mucosa

HIV patients have increased incidence of chronic HPV leading to an increased risk of cancer. To address the effect of HIV on HPV pathogenesis, we developed a mathematical model of HIV-HPV coinfection that captures known interactions such as decreased HPV-specific CTL and increase HPV production. We analyze the model and predict biological conditions under which coinfected individuals can clear HPV. We address the role of ART in coinfection and compare it to previous clinical observations.

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CP9

Identifying Hubs of the 2009 H1N1 Influenza Pandemic in the United States

A detailed data set captures incidence of influenza-like illness for 12 age groups in 825 US cities in 2009. A mechanistic mathematical model reproduces observed epidemic waves. Sites of long-distance transmission events are identified. These sites can be partly explained by autumn school onset. Basins emerge in which infection can be traced back to a jump site. These basins provide a testable hypothesis of the outbreaks phylogeography, bridging the gap between genetic and population surveillance.

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CP10

Machine Learning and Modeling: Are the Saguaro Cacti Dying Prematurely?

Bark injuries occur on the Saguaro Cactus in Tuscon, Arizona. These injuries are new with relatively few occurring prior to the 1950s. It is believed that UV-B rays due to climate change are at fault. Saguaros die as a result of extensive bark formation. We validate this claim mathematically using Machine Learning to predict the death of cacti due to barking and Statistical Modeling to illustrate that extant cacti will have a shorter lifespan.

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CP10

Eco-Epidemiological Model of the Salton Sea

Increasing levels of Salinity and outbreaks of botulism in Salton Sea are responsible for substantial mortality of pelicans and their prey,tilipia.A mathematical model for the population of both predator and prey proposed and its features analyzed. The dynamics of the system around each of the ecologically meaningful equilibria are presented.Natural disease control is considered before studying the impact of the disease in the absence of predators.

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CP10

Global Extinction Induced by Asymmetric Dispersal in Two-Patch Model with Allee Effect

We study asymmetric dispersal between two coupled populations under the Allee effect. With the Allee effect, initial populations below a threshold decline, while those above the threshold can persist. We explore the bifurcation structure while varying the dispersal rates and threshold. We show that there are no periodic orbits. At high Allee thresholds, we find large parameter ranges in which the globally extinct state is the only fixed point, even though uncoupled populations can persist.

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CP11

RNA Recombination Enhances Adaptability and is Required for Virus Spread and Virulence

While a high mutation rate fuels evolution, it also generates deleterious mutations. Recombination may resolve this paradox, alleviating the effect of clonal interference and purging deleterious mutations. Here we identified a poliovirus recombination determinant and generated a panel of variants with distinct mutation rates and recombination ability. We show, combining novel experiments and mathematical models, that recombination is essential to enrich the population in beneficial mutations and purge it from deleterious mutations.

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CP11

A Stochastic Two-Hit Model of Prion Disease

Prion diseases are characterized by a long lag-time where considerable time passes between the introduction of a prion particle and initial symptoms of the disease. There exists a rich literature of mass-action based mathematical models for this second phase, but little on stochastic models for the former. We present a stochastic "two-hit' model of prion disease and use it to answer questions about the rate of spontaneous disease initialization and explore the prion strain phenomenon.

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CP11

Modeling Treatment of RSV with TMC353121

Here we study the dynamics of respiratory syncytial virus treatment with TMC353121 using in vivo data from african green monkeys and a within-host mathematical infection model. We examine two different model formulations for the fusion inhibitor and compare how their predicted treatment outcomes differ. Using either model formulations, we find that TMC353121 has a maximum in vivo treatment efficacy of 75-80%.

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CP11

A Mathematical Model for the Interactions Between Plasmodium Falciparum Malaria Parasite and Host Immune Response

A new system of structured partial differential equations coupled with ordinary differential equations is established to investigate the population dynamics of Plasmodium falciparum and its interaction with red blood cells and cells of the immune system. A finite difference scheme is developed to solve the system. The newly developed model is applied to study the interplay between host immune response and parasite dynamics and investigate crucial experimental parameters for reliable prediction of treatment strategies.

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CP11

Extinction Pathways in a Stochastic Ebola Model

Zoonotic diseases, such as the Ebola virus disease (EVD), can be passed from an animal reservoir to a human host. There is little work devoted to understanding stochastic disease extinction and reintroduction in the presence of a reservoir. Here we build a stochastic model for EVD and explicitly consider the presence of an animal reservoir. Using a master-equation approach we determine the associated Hamiltonian, which we use to numerically compute the 12-dimensional optimal path to extinction.

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CP12

Triangulating Neurons: Spatial Localization via Extracellular Recordings

Extracellular recordings via multi-electrode probes are a basic tool in modern neuroscience. In principle, one can use these recordings to estimate the relative locations of neurons, potentially leading to applications including more accurate stimulation and spike sorting. However, in practice this is seldom done because of physical and technical constraints. Here, we analyze some sources of error in accurate spatial localization, and propose a Bayesian approach to the localization problem.

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CP12

Crowds as an Excitable Medium for Spiral Wave Dynamics

Spiral wave (SW) patterns are studied in many physical, biological, and chemical excitable systems. Of particular importance are SW of electrical activity that develop in the heart and give rise to arrhythmias such as tachycardia (single SW) and fibrillation (multiple SWs). We investigate if a crowd of people given simple rules for activation and deactivation, modeled on cardiac cells, can act as a living simulation for SW dynamics. For group sizes ranging from 50 to 650 people we demonstrate, experimentally, the existence of stable spiral waves and of spiral wave breakup leading to chaotic dynamics. Numerical simulation predicts the simple rules lead to well define wave fronts. People, however, respond with various degrees of anticipation and misinfor-

mation. This human behavior can lead to smoothed fronts or even lead to spiral wave breakup and chaos. We present a new cell model that includes variations in reaction to account for the observed behavior in crowds. This model may be useful in the study of coupling and decoupling of cardiac cells that lead to arrhythmic behavior.

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CP12

Bifurcation Analysis in the Hypothalamic-Pituitary-Adrenal Axis Including Gulcocorticoid Receptor Complex

The hypothalamic-pituiary-adrenal (HPA) axis plays an important role in the regulation of neuroendocrine and sympathetic nervous systems. Emerging evidence has shown that glucocorticoid act on glutamate neurotransmission system and consequently influences neuronal activities cognitive function. In this paper, we analytically derive the two parameter bifurcation analysis on one HPA model including Gulcocorticoid Receptor (GR) to explore the glucocorticoid bistability.

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CP13

Intervention Strategies for Epidemics: Does Ignoring Time Delay Lead to Incorrect Predictions?

We model how distributions of exposed and infectious periods affect disease spread. Ordinary differential equations allow a high probability of unrealistically short time periods, which could lead to inaccurate assessment of intervention strategies. Delay differential equations, which use fixed time periods, are more realistic but more difficult to analyze. Through steady state bifurcation analysis, we show that ODE models that work in the absence of control strategies can fail when quarantine is added.

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CP13

Modeling Transmission Dynamics of Ebola Virus Disease

Ebola Virus Disease (EVD) has emerged as a rapidly spreading potentially fatal disease. Several studies have been performed recently to investigate the dynamics of EVD. In this paper, we study the transmission dynamics of EVD by formulating an SEIR-type transmission model that includes isolated individuals as well as dead individuals that are not yet buried. Dynamical systems analysis of the model is performed, and it is consequently shown that the disease free steady state is globally asymptotically stable when the basic reproduction number, R0 is less than unity. It is also shown that there exists a unique endemic equilibrium when $R0 > 1$. Using optimal control theory, we propose control strategies, which will help to eliminate the Ebola disease. We use data fitting on models, with and without isolation, to estimate the basic reproductive numbers for the 2014 outbreak of EVD in Liberia and Sierra Leone.

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CP13

Fractional-Order SIR Models Derived from a Stochastic Process

Classic SIR models have been generalised to include fractional derivatives in order to capture a history effect. A large number of papers consider an ad hoc inclusion of fractional derivatives. This regularly leads to a violation of flux-balance and dimension disagreement. This talk addresses these problems in greater depth and considers the derivation of fractional order epidemic model as a stochastic process, solving the outlined problems.

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CP13

Investigating the Impact of Hiv and Malaria Co-Infection

We develop a semi-discrete epidemiology model to study the dynamics of HIV and malaria co-infection in a human population. Associated mono-infection models are derived and their dynamics are studied as a foundation for comparison with the complete model. Changes in individual disease dynamics resulting from disease interaction are the focus of study in the co-infection model. We seek what conditions create interactions sufficient to classify the co-infection as a syndemic.

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CP14

A Turing Model for Stereotypic, Space-Filling Lung Branching Morphogenesis

Organogenesis is a dynamic, self-organizing process. Many of the individual regulatory components, e.g. signaling molecules and their regulatory interactions, have been identified in experiments. However, an integrative mechanistic understanding of the regulatory processes is missing. Computational modeling provides a formalism to formulate and test hypotheses. We present and discuss a Turing model for the control of lung branching morphogenesis and focus on the numerical challenges in simulating the model on growing and deforming 3D domains. The 3D embryonic branching process can be recapitulated in the simulations. Further analysis of the model reveals fundamental properties of the Turing mechanisms that enable the stereotypic, reliable development of a space-filling lung tree.

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CP14

Efficient Parallel Simulation of Atherosclerotic Plaque Formation Using Higher Order Discontinuous Galerkin Schemes

Atherosclerotic plaque formation is today seen as a chronic inflammation of the arterial wall which grows over decades and may finally lead to a heart attack. The simulation of biological processes using partial differential equations may provide a deeper insight into this disease. After describing the mathematical model and the discretization scheme, we present some benchmark tests comparing commonly used DG methods. Furthermore, we take parallelization and higher order discretization schemes into account.

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CP14

Geometrical Constraints on Circulating Red Blood Cells

Red blood cells (RBCs) cleared from the bloodstream cannot be directly investigated, thus, maturation and elimination mechanisms are challenging to study. We take a geometrical viewpoint to connect the observed volume and surface-area of the circulating RBC population with the underlying physiology of RBC clearance. We propose that in order for an RBC with a fixed volume to go through a splenic-like slit the minimal surface area requirement during this passage can approximate the family of deformations by organizing the volume in the form of two spheres of equal radius, one sphere on each side of a splenic slit. This formulation provides a constraint on circulating cells: a volume-dependent minimal surface-area requirement must be met to allow the cell to complete this family of deformations and pass through a slit. Analysis of more than 100 human samples that include measurements of RBC volume and surface-area show that about 99% of RBCs obeying the two-sphere defined constraint, leaving 1% of cells candidates for clearance. The model and measurements demonstrate that collecting RBC surface-area distributions could be used in clinical setting to identify and quantify the RBCs deformability potential.

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CP14

Computational Model of Ventilator-Induced Lung Injury

Patients needing mechanical ventilation have air forced through the lungs to maintain their blood oxygen levels. This can cause strain-induced lung inflammation. We are developing a multi-scale model that accounts for airflow, tissue mechanics, and the cellular level inflammatory response. The inflammatory response is validated using cell experiments mimicking mechanical ventilation conditions and ventilated mice. These experiments and model are the first step in developing an understanding of ventilator-induced lung injury.

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CP15

Using Network Similarity Models to Address Challenges in Drug Development

Data-driven challenges in drug development are increasingly using graphical models to represent both biological processes as well as population-level trends. In this talk I will describe efforts that integrate heterogeneous biomedical data from pre-clinical and clinical data sets into network similarity models. We show that the resulting structure can lead to important conclusions about the efficacy of drugs at different stages of the drug development process.

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CP15

Model-Assisted Assessment of Aging and Hypertension on Cerebral Blood Flow Velocity

Both aging and hypertension have the ability to impair blood pressure regulation, making hypertensive elderly subjects particularly vulnerable to cerebral hypoperfusion and syncope during orthostatic stress. This talk proposes a simple nonlinear model that aims to describe and quantify the differences in dynamic cerebral autoregulatory response caused by aging and hypertension. Healthy young, healthy elderly, and hypertensive elderly human subject groups will be compared using model results via both *MATLAB* and *NONMEM*.

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CP15

Modeling the Effects of Body Mass Index on the Blood Concentrations of the Antibiotic Ertapenem

Ertapenem is an antibiotic commonly used to treat a broad spectrum of infections. A physiologically-based pharmacokinetic model was developed to investigate the uptake, distribution, and elimination of ertapenem following a once-a-day, single one gram dose. Parameters in the model that were not available in the literature were estimated using a least squares inverse problem formulation with published data for blood concentrations of ertapenem for normal height, normal weight males. Simulations were performed to consider the distribution of the antibiotic in underweight, normal weight, overweight, and obese men of varying heights.

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CP15

Uncovering Functional Relationships in Leukemia

Mass cytometers can record tens of features for millions of cells in a sample, and in particular, for leukemic cells. Many methods consider how to cluster or identify populations of phenotypically similar cells within cytometry data, but there has yet to be a connection between cell activity and other features and these groups or clusters. We use differential geometric ideas to consider how cell cycle and signaling features vary as a function of the cell populations. This consideration leads to a better understanding of the nonlinear relationships that exist in the cytometry data.

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MS1

The Impact of Shear Stress on Current Production and Structure of Electroactive Biofilms

Abstract not available.

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MS1

General Diffusion in Biological Environments

Complex fluids, the fluids with microstructures, are ubiquitous in biology. In this talk, I will concentrate on the study of ionic solutions through transmembrane proteins (ion channels). By employing a general energetic variational approach, the focus is on the coupling and competition between different mechanisms.

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MS1

A Multicomponent Phase-Field Model of Deformation and Detachment of a Biofilm under Fluid Flow

We present an energetic variational approach to model biofilm interaction with fluid flows. The biofilm is assumed an incompressible ternary mixture of viscous and viscoelastic fluids that represents bacteria, EPS and solvent phases. Our model satisfies an overall dissipative energy law and is solved with an efficient unconditionally energy-stable splitting scheme that is able to capture large-scale events of biofilm deformation and detachment under different hydrodynamic conditions, results that are qualitatively consistent with laboratory experiments.

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MS1

Deformation and Rupture of a Blood Clot under Flow Studied Using a Multi-Component Model

Diffusion interface (phase field) method is one of the most important approaches for studying multi-phase fluids due to its treatment of the interface as a physically diffuse thin layer. In this paper, the Energetic Variational Approach is used to derive a novel thermodynamically consistent model for the mixture of Newtonian and viscoelastic fluids. Elastic property of the viscoelastic fluid is described by the deformation gradient tensor in an Eulerian framework. Different densities and viscosities of distinct phases are taken into account. This new model is shown to satisfy the law of energy dissipation automatically. An energy stable numerical scheme is proposed to solve the coupled system of model equations. Numerical experiments are carried out to validate the model and the scheme for the problem with large density ratio and the problem with mixture of Newtonian and viscoelastic fluids. Specifically, the model is used to simulate the deformation of the blood clot under shear flow.

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MS2

Fibrin Gelation During Blood Clotting

A model of fibrin polymerization during blood clotting is formulated and a generatiing function approach for determining the model's behavior before and after gelation is developed. The model gives a mechanistic explanation for variations in gel structure (e.g., branch point density) seen experimentally. Explorations of the formation of fibrin gel under flow in response to a vascular injury are presented.

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MS2

Effective, General-purpose Multigrid Preconditioners for Implicit Immersed Boundary Methods

Implicit formulations of the immersed boundary (IB) method promise to improve the performance and robustness of the IB method by alleviating the severe time step restrictions of explicit IB methods, but most implicit IB methods use specialized solvers that are effective only for specific applications. We describe a multigrid approach to implicit IB formulations with general nonlinear structural models. Simple smoothers based on an approximate block factorization will be shown to be particularly effective.

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MS2

Modeling of Pulsating Soft Corals

Soft coral of the family Xeniidae have a pulsating motion, a behavior not observed in many other sessile organisms. We are studying how this behavior may give these coral a competitive advantage. We will present direct numerical simulations of the pulsations of the coral and the resulting fluid flow by solving the Navier-Stokes equations coupled with the immersed boundary method. Furthermore, parameter sweeps studying the resulting fluid flow will be discussed.

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MS2

Effects of Boundaries on Pulse Wave Simulations

Reduced order (1D) fluid dynamical models are useful tools for understanding the cardiovascular dynamics. Hemodynamic predictions in these models are known to be sensitive to the downstream boundary conditions, material properties of the conduit walls and the extent and topology of simulated network. In this talk, I will shed light on how different choices of boundary formulations and network topology could impact the hemodynamic simulations. I will also discuss the suitability of these choices for simulating physiological versus pathological hemodynamics.

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MS3

Polarization Generalized Poisson-Boltzmann and Poisson-Nernst-Planck Models

Abstract not available.

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MS3

Simulating Charge Transport in Ion Channels by a New Pnp Model

Abstract not available.

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MS3

Title Not Available

Abstract not available.

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MS3

Effects of (small) Permanent Charge and Channel Geometry on Ionic Flows via Classical Poisson-Nernst-Planck Models

Abstract not available.

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MS4

A Theoretical Model of Tissue Oxygenation in the Retina

The significance of impaired retinal tissue oxygenation to the pathophysiology of glaucoma is currently debated. Here, oxygen transport is simulated in a realistic microvascular network obtained from confocal microscopy images using a theoretical model that implements techniques from potential theory. Patient-specific values of pressure and arterial saturation are used to assess the effects of these factors on tissue oxygenation. Comparing model predictions with clinical oximetry maps demonstrates a role of blood flow in glaucoma.

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MS4

Optimal Control Strategies for Saccadic Eye Movements in Humans

In our investigations on eye motion, we used a generalization of Hill-type models of the musculo-tendon system for the lateral and medial recti. It is a eighth-order model with neural signals as inputs. The angle of the line of vision and the forces in the tendons are the outputs. To obtain the neural inputs, we set up two sequential optimal control problems. A Comparison of results with data from experiment (Robinson 1964) is presented.

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MS4

Influence of Tissue Viscoelasticity on the Optic Nerve Head Perfusion: A Mathematical Model

Proper perfusion of the optic nerve head (ONH) is vital to visual function. Alterations in ONH structures, like the lamina cribrosa (LC), have been associated with many pathologies, including glaucoma. We hypothesize that changes in LC viscoelasticity may compromise LC perfusion in response to sudden variations of intraocular pressure (IOP), possibly leading to disc hemorrhages. Due to difficulties in isolating these factors experimentally, we utilized a mathematical model to investigate IOP's influence on LC perfusion.

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MS4

Theory and Application of the LSPDE for Determining Gibbs Free Energies of Eye Lens Protein Mixtures

The Light-Scattering Partial Differential Equation (LSPDE) allows us to infer the Gibbs free energies of protein mixtures as functions of composition from light scattering data. We will present the basic theory of this fully-nonlinear, singular, degenerate elliptic equation. We will discuss well-posed problems and their relation to the practical determination of free energies. We will discuss computations, statistical methods for scattering experiments, and implications of this method for research into phase transitions associated with cataract.

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MS5

Inducing Alternans Using Delay-Differential Equations

Although electrical alternans, a state in which action potentials alternate between long and short, often precedes dangerous arrhythmias, many cardiac models do not

produce alternans. We show that incorporating delay-differential equations into an existing model can promote alternans development. We then analyze the behavior of the model voltage, currents, and gating variables to determine the effects of delays and how alternans develops in that setting. Finally, we discuss the implications of our findings.

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MS5

Calcium Alternans as a Critical Order-Disorder Transition

Electromechanical alternans is a beat-to-beat alternation in the strength of contraction of a cardiac cell, which can be caused by an instability of calcium cycling. Using a distributed model of subcellular calcium we show that alternans occurs via an order-disorder phase transition which exhibits critical slowing down and a diverging correlation length. We apply finite size scaling along with a mapping to a stochastic coupled map model, to show that this transition in two dimensions is characterized by critical exponents consistent with the Ising universality class. Finally, we discuss the effects of release refractoriness on the transition. These findings highlight the important role of cooperativity in biological cells, and suggest novel approaches to investigate the onset of the alternans instability in the heart.

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MS5

Period Doubling Cascade in Cardiac Tissue

Rapidly paced cardiac tissue readily displays alternans, a period-doubling bifurcation in electrical response, in which alternate beats have long and short responses despite a constant pacing period. While there are known mechanisms that describe these dynamics, no clear mechanisms exist to describe higher order periods. In this talk we present experimental evidence of higher order periods in cardiac tissue as well as a methodology to describe not only alternans in duration but alternans in amplitude as well as development of higher order periods.

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MS5

Spatiotemporal Dynamics of Calcium-Driven Alternans: Hysteresis, Multi-Periodicity, and Chaos

Numerous experimental and numerical studies have shown that calcium-driven cardiac alternans display novel dynamical behaviors not observed voltage-driven alternans. Furthermore, in some cases the effects of calcium-driven alternans may be more dangerous than voltage-driven alternans, both of which can precede ventricular fibrillation and heart failure. In this talk I will present a reduced model for calcium-driven alternans in a cable of tissue that captures many of the complex dynamics of real cardiac tissue but remains analytically tractable. Confirmed by simulations of complex ionic models, the model predicts many novel dynamical states, including standing and traveling waves, hysteretic discontinuous patterns, and states with simultaneous multiple periodicities and chaos. The hysteretic discontinuous state admits a novel phenomenon where nodes, i.e., phase reversals, can be pulled towards the pacing site via a change in parameters, but cannot be pushed away - a phenomenon we call unidirectional pinning. At more extreme parameter values these states undergo a complex series of bifurcations resulting in multiple coexisting dynamical states along the cable, including periodicities of different orders and chaos. In each case our reduced model can be used to explain the particularities of these dynamical states.

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MS6

Stochastic Models for the Stem Cell Niche

Abstract not available.

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MS6

Stochastic Modeling of Yeast Cell Polarization: From Cell Budding to Population Development

Abstract not available.

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MS6

Multi-Step Transitions Between Epithelial and Mesenchymal States and Cellular Plasticity

Abstract not available.

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MS6

Find Network Topologies That Can Achieve Biochemical Adaptation and Noise Attenuation

Abstract not available.

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MS7

To Infer Network Connectivity, What Measurements Must Be Made?

We develop methods of nonlinear data assimilation in order to identify the measurements required to obtain predictions of a complete model of a dynamical system. The procedure involves providing an optimization algorithm with measurements, and obtaining estimates of all state variables (both measured and unmeasured) and all parameters. In this context, we are determining what information about network properties is contained in the voltage time series output of the neurons within that network, and the fraction of neurons in a network that are required.

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MS7

Neural Models and Their Interactions in the Song Center of the Zebra Finch

The male zebra finch learns to sing its song by listening to a tutor bird, typically its father. The neural "song center" for this behavior, the HVC, has been identified. In vivo electrical recordings from neurons of the HVC reveal a sparse neural coding, whereby HVC projection neurons produce bursts of action potentials at a precise time during each rendition of the song. In vitro electrical recordings are being used to determine the ion channels present in the neurons and their contribution to the spike pattern. In this presentation I discuss work we are doing to integrate these data, using mathematical modeling and the Dynamic Clamp technique.

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MS7

Learning Effects on Somatic Ionic Currents

The currency of neuronal communication is spike timing. We discovered a novel mechanism for regulating spike timing while making intracellular recordings in nucleus HVC of the songbird. Within each bird, all neurons share similar timing features, they varied across birds, and were strikingly similar among siblings. Exposing birds to delayed auditory feedback changed the waveforms dramatically. This represents the first example of a fast physiological signal that carries feedback error information in birdsong learning.

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MS7

Robustness in a Rhythmic Neuronal Circuit

How can networks formed from variable neurons with disparate intrinsic and synaptic conductances be robust? We study this problem experimentally and computationally and explore simple control rules that allow neurons to find solutions that are robust to perturbation by environmental conditions and neuromodulation.

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MS8

Enumerative Properties of Gene Tree Configurations in Species Trees

Computation of the conditional probability of a gene tree given a species tree can be performed by algorithms that use certain combinatorial structures to describe the possible configurations the gene tree can assume inside the branching structure of the species tree. These structures include *coalescent histories* and *ancestral configurations*. In this talk, we use these structures to present several enumerative, asymptotic and bijective results considering gene trees and species trees with a matching topology.

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MS8

Branching Polytopes: Geometric Combinatorics and RNA Secondary Structures

The Nearest Neighbor Thermodynamic Model (NNTM) computes the free energy of an RNA secondary structure as the sum of the free energy of smaller substructures. Many of the parameters used to predict the free energy of the substructures are experimentally determined, but those pertaining to the free energy of multiloops are not.

This talk will discuss recent work using linear programming and computational geometry to analyze these parameters.

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MS8
Local Equations for Equivariant Evolutionary Models

Phylogenetic varieties related to equivariant substitution models have been studied largely in the last years. One of the main objectives has been finding a set of generators of the ideal of these varieties, but this has not yet been achieved in some cases (for example, for the general Markov model this involves the open "salmon conjecture") and it is not clear how to use all generators in practice. However, for phylogenetic reconstruction purposes, the elements of the ideal that could be useful only need to describe the variety around certain points of no evolution. With this idea in mind, we produce a collection of explicit equations that describe the variety on a neighborhood of these points. Namely, for any tree on any number of leaves (and any degrees at the interior nodes) and for any equivariant model on any set of states, we compute the codimension of the corresponding phylogenetic variety. We prove that this variety is smooth at general points of no evolution, and provide an algorithm to produce a complete intersection that describes the variety around these points.

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MS8
Parametric Analysis of RNA Secondary Structure Prediction

The problem of predicting the structure of the RNA molecule is an important problem in computational biology. Thermodynamics based methods depend on an energy function that uses hundreds of parameters, while language theoretic approaches depend on probability parameters derived by training grammars. We will discuss our findings on the parametric analysis of some of the models that are used, focusing on a grammar based method.

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MS9
Modeling Rhythmic Biological Behaviors Using Limited Data

A staggering diversity of biological and engineered systems exhibit rhythmic behaviors, and their dynamics have been analyzed for hundreds of years. Yet, data-driven modeling and analysis of rhythmic behaviors remains in its infancy and such tools are essential for understanding systems for which "first-principles" models are not feasible. Identifying the dynamics of rhythmic systems from input–output data is critical to many applications in robotics and biology, and yet remains a challenge. Here, we describe a new formulation for identifying rhythmic dynamical systems by using harmonic transfer functions. This formulation side-steps the well-known problem of estimating the limit cycle itself, enables separate identification of input and measurement delays, and applies to both hybrid and continuous dynamical systems. An important feature of our work is the selection of effective stimuli when large numbers of oscillatory cycles cannot be easily obtained. We present preliminary results on the application of these techniques to the identification of muscle dynamics in experiments involving *ex vivo* lamprey muscle.

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MS9
Effects of Sensory Feedback on Lamprey Locomotion

Mechanoreceptive neurons called edge cells, located on the margin of the spinal cord in lampreys, are known to respond to stretch and provide sensory information directly to the central pattern generator (CPG). Using experimental data from bending experiments on the lamprey spinal cord, we classify unit responses using spike-triggered averages and phase dependent impulse response to give us insight into how to model proprioceptive sensory feedback in closed-loop swimming.

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MS9

The Neural Mechanisms of Limb Coordination in Crustacean Swimming: The Roles of Nearest-Neighbor and Longer-Range Connectivity

During forward swimming, long-tailed crustaceans rhythmically move 4-5 pairs of limbs in a back-to-front metachronal wave with inter-limb phase-differences of $\sim$ 25% over the entire range of behaviorally-relevant stroke frequencies. Recently, we showed that this limb coordination provides near optimal swimming efficiency. The neural circuit underlying limb coordination can be viewed as a chain of coupled oscillators. We describe how the circuit architecture provides a robust mechanism for coordination,specifically discussing the roles of nearest-neighbor and longer-range connectivity.

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MS9

System Identification of Free Flight Maneuvers in Agile Insects

Animals demonstrate remarkable stability and maneuverability in complex environments. These behaviors emerge from the closed-loop, feedback interactions between neural and mechanical physiological systems. I will discuss how we can alter this feedback structure in experiment and analysis in order to make testable predictions about animals neuromechanical systems. Our system identification approach reveals how hawk moths, agile flying insects that hover in exceptionally low light, process visual information and stay aloft in challenging environments.

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MS10

Data Analysis and Mathematical Modeling of Multiscale Dynamics in Human Cortex

Epilepsy is a life-shortening brain disorder affecting 3 million people in the United States. Motivated by recordings from human subjects, we are developing a computational modeling framework to simulate the ionic and neuronal mechanisms that govern spatiotemporal dynamics during spontaneous seizures. Model observables are constrained to match data recorded from standard clinical electrodes and microelectrode arrays implanted in human patients. Our most recent work focuses on the spatiotemporal patterns that emerge during human seizure.

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MS10

The Contribution of Interneurons to Hippocampal Oscillations

How interneurons contribute to the generation of oscillations in the hippocampus remains unclear. For interneurons recorded in mice hippocampal CA1 area, by using time-delayed mutual information, we identified two subsets of interneurons whose firing activities share high mutual information with theta-band (4-12 Hz) and ripple-band (100-250 Hz) LFP signals, respectively. Information flow direction further suggests their unique contribution to theta and ripple oscillations. Finally, we emphasize that Granger Causality analysis may fail in this case.

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MS10

Spike-Triggered Regression on Neuronal Network Reconstruction

We propose a spike-triggered regression (STR) method to accurately reconstruct the network connectivity of a nonlinear integrate-and-fire (I&F) neuronal network. The basic idea of our method is to capture the subthreshold voltage response to a presynaptic spike through linear regression. Through numerical simulations, we demonstrate that, by using relatively short-time recordings, the I&F neuronal network connectivity can be well reconstructed using our STR method.

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MS10

Sparsity and Compressed Coding in Sensory Systems

Considering that many natural stimuli are sparse, can a sensory system evolve to take advantage of this sparsity? We model an early sensory pathway using an idealized neuronal network comprised of receptors and downstream sensory neurons. By revealing a linear structure intrinsic to neuronal network dynamics, our work points to a potential mechanism for transmitting sparse stimuli, related to compressed-sensing (CS) type data acquisition and the impact of localized receptive fields beyond conventional CS theory.

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MS11

Using Kalman Filtering for Prediction of Cardiovascular Regulation During Blood Withdrawal

To analyze baroreflex regulation during blood withdrawal, we develop a patient-specific cardiovascular circulation model predicting pressure and flow in a 0D network analogous to an RC-circuit. Blood withdrawal is modeled from an experimental procedure used to obtain pressure and volume measurements in the left ventricle of healthy Sprague Dawley rats. We employ Kalman filtering to estimate and quantify uncertainty relating to time-varying quantities controlled by the baroreflex, including peripheral resistance, cardiac contractility, and venous compliance.

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MS11

Integrating Model-Free and Mechanistic Modeling Approaches for Parameter Estimation and Prediction

The ability to make accurate predictions of the system state is of great interest in the life sciences. Mathematical models, parameterized by a number of unknown parameters, have been used for this purpose. In contrast nonparametric prediction methods exist, relying solely on historical data from which to build predictions. Both approaches offer advantages as well as significant limitations. In this talk, we consider a hybrid scheme which utilizes the complementary features of both.

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MS11

Estimating Kinetic Rates of Prion Replication from a Structured Population Model

Prion proteins cause a variety of fatal neurodegenerative diseases in mammals but are harmless to yeast, making it an ideal model organism for these diseases. Determining kinetic parameters of prion replication in yeast are complicated because experiments reflect both the disease and yeast population dynamics. We present a structured population model describing the distribution and replication of yeast prions in a population of cells. I employ the Prohorov metric to estimate kinetic parameters from experiments.

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MS11

Parameter Estimation in Modeling Influenza Infections: When and Why Parameter Values Don't Matter

Relatively little is known about the rates of virus infection and clearance. Estimating these rates by fitting a kinetic model to viral load data often results in parameters that are correlated and/or non-identifiable. While this may seem problematic, robust predictions are still possible. I will discuss why parameter behavior is more important than specific values and give an example of how a parameter value may be accurate even when its correlated to other parameters.

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MS12

Pancreatic Beta Cells - Synchronization and Intrinsic Heterogeneity

Human pancreatic beta cells are known to synchronize in phase. We investigate the underlying mechanisms behind this synchronization and the role of heterogeneity in the intrinsic properties of the individual cells on network activity. Non synchronous behaviors are explored, and we will consider their causes and meanings both mathematically and biologically. We will use modeling, simulations, and dynamical systems tools to drive our understanding of beta cell synchronization and insulin production.

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MS12

Glucose Oscillations Can Activate An Endogenous Oscillator in Pancreatic Islets

When stimulated by glucose, pancreatic islets release insulin in pulses governed by an endogenous oscillator. As glucose rises to excessive concentrations, it crosses a threshold above which the islet oscillator is silenced and pulsatile release is lost. We demonstrate, using mathematical modeling and experiments with islets in a microfluidic device, that lost oscillations can be recovered by a sinusoidal glucose stimulus. We explain how our results support the existence of bistability in the islet oscillator.

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MS12

Applying Mathematical Modeling to Drug Development Decisions: Non-Clinical and Phase I Evaluation of Hypoglycemic Risk of a Novel, Partial Glucokinase Activator

PF-04937319 (PF-319) is a novel small molecule glucokinase partial activator (GKA) for the treatment for type 2 diabetes. While this drug class offers potential for controlling hyperglycemia, several GKAs were discontinued for hypoglycemia. Mathematical modeling was utilized at several stages of PF-319's development to understand and mitigate safety liabilities. We present two case studies for PF-319: a non-clinical study to increase confidence-in-rationale and an analysis of several pharmacokinetic formulations designed to reduce hypoglycemia.

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MS12

Alpha-Cell Heterogeneity: The Role of TASK

Understanding the mechanisms involved in regulating glucagon secretion from the pancreatic α-cell has proven to be quite difficult. Currently, there are many plausible theories involving intrinsic and paracrine regulation. We suggest that the variety of data is a consequence of heterogeneity and use a simplified model to test whether heterogeneity can account for these diverse observations. In particular, we investigate the importance of TASK-1 in regulating glucagon secretion and overcoming the innate heterogeneity of α-cells.

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MS13

Generating a Large Cohort of Virtual Patients - An Application to a Complex PDE Model for Erythropoiesis

Adequately expressing inter-subject variability in virtual patient cohorts is crucial for critical hypothesis testing to fill key knowledge gaps in our understanding of complex physiological systems. However, the constrained nature of clinical measurements makes the estimation of large sets of parameters in comprehensive mathematical models sometimes unfeasible. We present a novel data driven physiologically informed approach to construct large cohorts of virtual patients that meet a-priori stimulus-response constraints.

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MS13

Inverse Problems and Parameter Estimation in the Era of Precision Medicine

"Precision Medicine' requires that treatment strategies are based on individual properties of the patient. We concentrate on the situation where a mathematical model is the basis for the proper therapy. This demands to determine the key parameters of the model which capture the individual properties of the patient. Consequently we need powerful methods for all aspects of parameter estimation on the basis of available data.

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MS13

Computation of Optimal Epo Doses for Patients with Chronic Kidney Disease Using a Model Predictive Control Approach

We present a nonlinear model predictive control (MPC) approach for the computation of optimal erythropoietin (EPO) doses, that are administered at specific time instances. MPC offers the possibility to account for bleedings and wrong administered doses within the optimization process. Numerical results for a variety of dialysis patients are computed by using a projected BFGS method and we analyze the effect of restricting EPO doses to be constant over a number of administrations.

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MS13

A Structural Model of Passive Forces in Myofibrils Allowing Efficient Parameter Estimation

Passive forces in myofibrils of striated muscles are mainly related to the giant protein titin. There is a strong body of evidence that muscular diseases like dilated cardiomyopathy are related to altered expressions of titin isoforms. We analyze a stochastic model of passive force production in stretched myofibrils which takes into account the force dependent unfolding and refolding of titins immunoglobulin domains and introduce a method allowing for efficient parameter estimation of titin properties.

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MS14

Stochastic Features of Airway Liquid Flows

The liquid lining of lung airways has an important role in defense and in regulating airway stability. It has complex constitutive properties and it coats a surface with elaborate geometrical form. Here we investigate how random spatial heterogeneity, of the film itself and of the substrate on which it sits, influences the film's configuration and flow properties. We exploit low-order models, exploiting underlying physical balances, to characterize distributions of flow features.

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MS14

Causes and Effects of Material Heterogeneity in Biofilms

Abstract not available.

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MS14

Stochastic Modeling of Cancer Cell Lineage with Time Delays

Abstract not available.

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MS14

Strong Defense by Weak Affinities: Modeling Virus-Antibody-Mucin Kinetics

A promising strategy to reduce HIV transmission is to design antibodies (Ab) that can crosslink HIV to mucins comprising cervicovaginal mucus (CVM), thereby blocking viruses from reaching and infecting target cells. Here, we modeled the kinetics of HIV in semen that diffuse into CVM populated by Ab with distinct affinities to mucins. We compared a continuum approach using partial differential equations for the diffusion of Ab and virion concentrations with stochastic simulations of individual virions.

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MS15

Computational Modeling of a Swimming Lamprey Driven by a Central Pattern Generator with Sensory Feedback

The lamprey is a model organism for both neurophysiology and locomotion studies. We present a computational swimming lamprey driven by a central pattern generator

(CPG) modeled as a chain of coupled oscillators. The CPG drives muscle kinematics in fluid-structure interactions implemented in an immersed boundary framework to produce the emergent swimming mode. Body curvature changes provide feedback to the CPG. Effects of feedback to the neural activation on swimming performance are estimated and examined.

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MS15

Stochastic Fluctuations in Suspensions of Swimming Microorganisms

Abstract not available.

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MS15

They Are Not Third-Parties: Solutes and Polymers in the Fluid-Structure Interaction

The immersed boundary method is considered in two contexts: I) solutes around water semi-permeable membranes mediate in the fluid-structure interaction. With chemical potential barriers, membrane electrophysiology and osmotic swelling are well realized while interface conditions are removed. II) polymeric complex fluids in the fluid-structure interaction are represented by non-Newtonian two-phase medium. In the *C. elegans* swimming, generation of hyperbolic points and swimming speed retardation are elucidated by the extensional flow and stretching/compression of polymers.

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MS15

Self-Organization in Micro-Swimmer Suspensions

Self-organization of micro-swimmers such as bacteria into intricate patterns is known to happen in nature and has also been observed in many experiments. In the absence of external stimuli or quorum sensing, this self-organization of the colony occurs due to mechanical contact and hydrodynamic forces between the individual bacteria and is guided by the confinement geometry. We will explain a mathematical model and direct simulation method that captures the correct individual and collective dynamics. The dynamics of micro-swimmers inside circular drops, long micro-channels as well as peristaltic domains will be discussed.

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MS16

Membrane Mechanics and the Influence of Integral Proteins: Continuum Elasticity Theory and Proteins of Arbitrary Shape

Biological membranes deform in response to resident proteins leading to a coupling between membrane shape and protein localization. Additionally, the membrane biophysical properties influence the conformation and function of membrane proteins. While it has been argued that continuum elastic models for the membrane cannot reproduce the distortions observed in fully-atomistic molecular dynamics simulations, we suggest that this failure can be overcome by using chemically and geometrically accurate representations of the protein. We present a hybrid continuum-atomistic model that uses a novel finite volume solver to find the minimum energy equilibrium of the membrane-protein system. Our numerical approach allows for distortions of the grid representation of the membrane near the protein leading to smooth and more realistic membrane-protein boundaries. We show the model is in excellent agreement with fully-atomistic simulations of many systems: gramicidin, Gltph and nhTMEM16 lipid scramblase. Thus, the speed and accuracy of continuum-atomistic methodologies allow for the modeling of long length-scale, slow experimental processes, such as membrane morphological changes, that are currently beyond the scope of other computational approaches.

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MS16

Fluctuating Vesicles in a Time-Dependent Viscous Flow

We study the nonlinear, nonlocal dynamics of two-dimensional vesicles in a time-dependent, incompressible viscous flow at finite temperature. We focus on a transient wrinkling instability that can be observed when the direction of applied flow is suddenly reversed. Using a stochastic immersed boundary method with a biophysically motivated choice of thermal fluctuations, we find that thermal fluctuations actually have the ability to attenuate variability of the characteristic wavelength of wrinkling by exciting more wrinkling modes.

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MS16

Composition Induced Bifurcation in Multicomponent Lipid Membranes

Lipid bilayers are composed of a multitude of lipid constituents, and their distribution over the inner and outer leaflets of the plasma membrane are known to have predetermining influence on membrane curvature and endocytotic events. We present a 'minimal' continuum model of lipid membranes that supports families of bilayer morphologies, allows for bifurcation to higher co-dimensional morphologies, such as filaments and micelles, and provides for a rich mathematical competition between intrinsic curvature and morphological evolution. We identify structure that inhibits the bifurcations, rendering large families of bilayers intrinsically stable, while affording coupled evolution of bilayer composition and morphology. We present motivating examples from the endoplasmic reticulum.

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MS16

High-order Boundary Integral Algorithms for Vesicle Flows

We present fast schemes for the high-fidelity simulation of suspensions of vesicles in 3D Stokes flow. The vesicles' shapes are evolved as a result of interplay between bending and tensile interfacial forces, hydrodynamic interaction between vesicles, as well as the fluid flow, which is governed by Stokes equation. Simulations of such flows require algorithms for highly stiff, nonlocal, and nonlinear interfacial forces. Semi-implicit time stepping schemes coupled with spectral representation of the surface.

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MS17

Modeling Contact Lens Motion and Tear Film Dynamics During Blinking

We develop a mathematical model that couples the dynamics of the tear film and contact lens during blinking. We derive an ordinary differential equation for the motion of the contact lens (parallel to the cornea) driven and retarded by viscous forces in the thin fluid films separating the contact lens from the eyelids and the corneal surface. The lens and lid motion influence the tear film dynamics.

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MS17

Tear Film Dynamics on a Model Blinking Eye-Shaped Domain

By composing a stretching map with a conformal map, a square domain can be transformed into one that resembles a human eye. Rectangular sections of the domain also resemble the eye in various stages of closing. These observations allow a straightforward and spectrally accurate numerical method to run simulations on the eye surface as it blinks. The idea is demonstrated for some 2nd and 4th order PDEs with Dirichlet and no-flux conditions.

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MS17

Modeling Contact Lens Induced Suction Pressure

We study the mechanics of contact lenses to understand how lens design affects patient comfort. When a contact lens is placed on an eye, it is deformed and this deformation induces stresses. These stresses induce a suction pressure distribution in the tear film. We present a model that predicts the suction pressure and we explore the influence of that pressure on corneal deformation.

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MS17

Tear Film Evaporation and Breakup with a Mobile

Lipid Layer

Tear film breakup (TBU) can cause irritation and damage to the eye, motivating research to understand and prevent TBU. We apply lubrication theory to model the tear film as a system of two mobile fluid layers, the aqueous and lipid layers, and analyze potential causes of local TBU. We analyze a variety of physical situations and compare the results of our model to local breakup as observed in experiments. Supported by NSF DMS 1412085.

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MS18

Floquet Stability Analysis of a Model of Two-Dimensional Paced Cardiac Tissue Exhibiting Wave Breakup

For a two-dimensional layer of cardiac tissue, an increase in the pacing frequency induces a period doubling bifurcation (alternans) with further increase producing wave breakup associated with lethal arrhythmias. We present the Floquet analysis of period-doubled solutions of a tissue model reproducing this experimentally observed behavior. In particular, we discuss the implications of the structure of the adjoint eigenfunctions on the wave breakup and on our ability to suppress it using feedback control.

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MS18

Subcellular Spatiotemporal Calcium Dynamics Underlying Early Afterdepolarizations in Ventricular Myocytes

We discuss novel insights into the dynamical origin of early afterdepolarizations (EADs) in the setting of the long QT syndrome, an inherited life-threatening heart rhythm disorder caused by mutations of cardiac ion channel genes. The study makes use of a physiologically detailed mathematical model that accounts for the spatially distributed and stochastic nature of calcium release from intracellular stores as well as the bi-directional coupling of calcium and voltage dynamics. The results highlight the importance of subcellular calcium dynamics in the genesis of EADs and are in good agreement with experiments.

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MS18

Characterization of Spatial-Temporal Chaos in Excitable Media and Transitions Between Chaotic and Non-Chaotic States

Cardiac tissue as an excitable medium exhibits a rich diversity of dynamical patterns, including spiral waves and spatial-temporal chaos, which can be associated with cardiac arrhythmias. The distinction whether the underlying dynamics is governed by an actual chaotic attractor or is more of a transient nature could improve the understanding and the control of arrhythmias. Here we characterize the chaotic dynamics using Lyapunov exponents and investigate the transient behavior of such systems.

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MS18

Spatial Discordance and Phase Reversals in a Discrete-Time Map Model

Alternans is an arrhythmogenic beat-to-beat alternation in the cardiac action potential duration (APD). Using a discrete-time map model, I analyze the stability of a propagating electrical wave in a one-dimensional cardiomyocyte model during an alternating heart rhythm. Analytical expressions are derived to predict APD phase reversals, identifying dimensionless parameters that govern the transition from spatial concordance to discordance. Finally, theoretical predictions are shown to agree closely with numerical simulations of an ionic myocyte model.

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MS19

Robust Dynamics in Tissue Growth and Stochastic Developmental Patterning

Abstract not available.

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MS19

Stochastically Patterning the Early Mammalian Embryo

Abstract not available.

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MS19

Comparison of Stochastic and Deterministic Models of Cell Polarity

Abstract not available.

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MS19

Energy Landscape and the Two-Scale Large Deviations for Biological Stochastic Dynamics

Abstract not available.

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MS20

Phase Oscillator Model of Insect CPGs

CPGs are networks of neurons in the spinal cords of vertebrates and invertebrate thoracic ganglia, capable of generating muscular activity in the absence of sensory feedback. A mathematical model of the CPG in cockroaches describes the behavior of a fast nonlinear current, a leakage current, a slow potassium current and a very slow calcium-mediated current found in bursting neurons (BN). A mathematical technique, called phase reduction, reduces the complex set of bursting neurons to 6 coupled nonlinear phase oscillators, each corresponding to a neural network controlling one leg. First, we provide an overview of the BN models and their phase reductions using PRCs. Next, we discuss the resulting insect gaits and their stability properties.

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MS20

How Does the Brain Generate Sequences for Behavior?

Sequential activity of neural ensembles has been observed during a range of computations, but the circuit mechanisms underlying the generation of these sequences is poorly understood. In the zebra finch, a cortical circuit critical for song production forms a sequential pattern of premotor bursts that ultimately drive the muscles producing the song. Here we use anatomical and physiological methods to investigate their interconnectivity within HVC and to test hypotheses concerning the origin of higher order population dynamics within this region.

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MS20

Dynamical Systems Models of Songbird Singing

In a collaboration with Gabriel Mindlin (Univ. Buenos Aires) we have developed and experimentally tested models of learned vocal movements (peripheral vocal and respiratory muscles) songbirds make when singing. We observe correspondence between model dynamics and activity patterns of forebrain "HVC" neurons (that are important for generating timing information). A second model describes patterned activity throughout the forebrain, midbrain, and brainstem. Collectively, these results promote analysis of motor control in a nonlinear dynamical systems framework.

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MS20

Scientific Applications of Bayesian Event Time Inference

Timeseries data in neuroscience (calcium imaging, electrophysiology, etc.) often consist of events and noise. We can use Bayesian tools to find times of events, event dynamics, and model parameters. To analyze imaging data from songbirds, we have leveraged multiple trials of stereotyped neural activity to perform temporally precise inference. In other settings, extensions to the basic event inference allow for artifact removal, fusion of different modalities (calcium imaging and electrophysiology), or model comparison.

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MS21

A Stochastic Algebraic Model of Synergistic T Cell Activation by Pharmaceutical Agonists

In this talk, a stochastic algebraic model is presented of T cell stimulation for cancer immunotherapy with two pharmaceutical agonists found to have a synergistic effect on T cell function *in vitro*. A polynomial dynamical system (PDS) is used to analyze a deterministic model of the perturbed intracellular network. A stochastic component associated with the update rules of the PDS is added and the resulting system is used to help explain T cell activation synergy.

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MS21

A Boolean Network Model of the L-Arabinose Operon

In genetics, an operon is a segment of DNA that contains several co-transcribed genes, which together form a functional regulatory unit. Operons have primarily been studied in prokaryotes, with both the lactose (*lac*) and tryptophan (*trp*) operons in *E. coli* having been classically modeled with differential equations and more recently, with

Boolean networks. The L-arabinose (*ara*) operon in *E. coli* encodes proteins that function in the catabolism of arabinose. It differs from the *lac* and *trp* operons in that it exhibits both positive and negative gene regulation within a single operon. In this talk, I will describe our proposed Boolean network model for the *ara* operon, which consists of both a physical wiring diagram, and the logical functions that govern each node. I will also describe the results of model validation and current and future research.

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MS21

Weakly Mutually Uncorrelated Codes

We introduce the notion of weakly mutually uncorrelated (WMU) sequences, motivated by applications in DNA-based storage systems and synchronization protocols. WMU sequences are characterized by the property that no sufficiently long suffix of one sequence is the prefix of the same or another sequence. In addition, WMU sequences used in DNA-based storage systems are required to have balanced compositions of symbols and to be at large mutual Hamming distance from each other.

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MS21

Toric Ideals of Neural Codes

A neural code is a collection of firing patterns of a set of neurons; it is convex if there exists a realization using convex open sets where each codeword corresponds to a region in the arrangement. While some methods exist to determine whether a neural code is convex, these methods do not describe how to draw a realization. We use toric ideals, along with the theory of piercings, to draw realizations for particular classes of codes.

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MS22

Neural Control of Leg Movements in Drosophila

To execute appropriate movements, the nervous system must not only integrate multiple streams of sensory information and make behavioral decisions, it also must recruit complex multi-jointed limbs in the correct order. Owing to its size and complexity, computations underlying sensorimotor transformations are difficult to understand in the mammalian brain. We present recent advances we have made in studying sensorimotor transformations in Drosophila. The talk will focus on the control of leg movements in Drosophila.

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MS22

Towards a Biomechanical Template for Slow Walking

Legged locomotion is complex: it requires precise coordination amongst multiple joints within a limb and coordination between limbs. However, many approaches to legged locomotion employ simplified approaches aimed at understanding basic principles underlying locomotion rather than the detailed dynamics of each joint and limb which may be especially useful to understand neuro-mechanical coupling and environmental influences. We will present a biomechanical template to describe slow walking and test our model with data from fruit flies.

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MS22

Neuromechanical Control of Jellyfish Turning

In order for an organism to have an effective mode of locomotion, the underlying neuromuscular organization must be capable of controlling maneuverability in a changing environment. In scyphomedusae, the activation and release of muscular tension is governed by the interaction of the pacemakers with the underlying motor nerve net that controls the musculature. The pacemaker can respond to environmental cues from the diffuse nerve net and adjust their firing frequency. This distributed control mechanism in turn allows one pacemaker to set the pattern of the bell's muscular contraction. To turn, a pacemaker on the inside of the turn must actively fire and induce asymmetrically timed contraction in the rest of the bell. In this work, we explore the control of neuromuscular activation with a model jellyfish bell immersed in a viscous fluid and use numerical simulations to describe the interplay between active muscle contraction, passive body elasticity, and fluid forces. The fully-coupled fluid structure interaction problem is solved using an adaptive and parallelized version of the immersed boundary method (IBAMR). This model is then used to explore the interplay between pacemaker firings, fluid dynamics, and the mechanical properties of the bell.

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MS22

Spike Trains to Force Generation

Muscle contraction occurs when neuron action potential stimulate the sarcoplasmic reticulum, releasing calcium ions that then bind to muscle filaments, allowing the myosin to contract the muscle. I will present a model that couples spike-train activation to mass-action equations for calcium ions, which in turn couples to the Hill model for muscle contraction force-velocity relationship. This model allows for investigation of spike trains required to produce partial twitch response, and total tetanic contraction.

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MS23

The Progression of Parkinson's Disease in the Basal Ganglia

Muscle rigidity associated with Parkinsons disease (PD) is thought to be correlated with the loss of dopamine and the emergence of beta oscillations in the basal ganglia. As dopamine-producing neurons die off, synaptic connection strengths change leading to favoring of specific pathways. Modeling a healthy basal ganglia and then a PD basal ganglia we can show the disease progression and which connections are to blame, as this is still under debate in the scientific community.

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MS23

The Role of Gap Junctions Between Excitatory Neurons in the Cortex

Researchers believe that electric coupling through gap junctions may facilitate the emergence of global oscillations in the brain. Fitting data from experimental papers, we construct a detailed model with synaptic and electric coupling using a modified version of the Hodgkin-Huxley equations. We use this model to examine the dynamical regimes that emerge though the incorporation of both electric and synaptic connections, with a specific interest in the emergence and properties of synchrony.

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MS23

Deep Brain Stimulation in the Subthalamic Nucleus Can Restore Function in Striatal Networks: A Modeling Study

Parkinson's disease is associated with high power in the alpha/beta (8-30Hz) frequency range, and deep brain stimulation (DBS) reduces power in those rhythms, leading to better motor function. We use computational models to show that, unlike other theories of how DBS works, high frequency DBS can normalize activity in the striatum, a portion of the basal ganglia from which the pathological rhythms may arise. By contrast, low frequency DBS creates resonance for the pathological oscillations.

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MS23

Pallidostriatal Projections Promote Beta Oscillations Under Dopamine Depletion

Recent experimental findings suggest a role for an inhibitory loop in the basal ganglia, called the pallidostriatal circuit, in generating activity patterns associated with parkinsonian dopamine depletion. We present a new ODE model of this network and discuss its dynamics under normal and diseased conditions, highlighting the mechanisms underlying the emergence and amplification of rhythmicity and synchrony. Interesting aspects include the transmission of rhythmicity through a node lacking rhythmic activity, via induction of rhythmic pauses.

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MS24

Modeling Time Series of Composite Disease Activity Indices

Disease status is often expressed using composite indices that combine multiple characteristics into a single score. The index components may respond to a treatment in different ways, making it difficult to translate results across study designs. Here, we describe a Bayesian method for a modeling the stochastic dynamics of disease indices within a study population. We show that capturing the dynamics of composite indices improves study interpretation and provides actionable information for study design.

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MS24

Towards a Model-based Control of Neuronal Systems

Observability of a dynamical system requires an understanding of its state. However, existing techniques are too limited to measure all but a small fraction of the physical variables and parameters of neuronal networks. We constructed models of the biophysical properties of neuronal membrane, synaptic, and microenvironment dynamics, and incorporated them into a model-based predictor-controller framework. Our results render the incorporation of the dynamic microenvironment in neuronal models a key for successful tracking of pathological states.

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MS24

Development of the MCR Method for Parameter Estimation in Continuous-Time Markov Chain Models

Parameter estimation techniques have been successfully and extensively applied to deterministic models but are in early development for stochastic models. In this talk, we introduce a new method, the MCR method, for approximating parameters for a continuous-time Markov chain (CTMC) model. Comparing this method to an established method, the MCR method provides significantly better estimates and smaller confidence intervals for parameter values on the two example models considered.

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MS24

A Mathematical Model of Gl261-Luc2 Glioma Growth in Mice

Five immune-competent mice were injected with GL261-Luc2 cell line, mimicking human strains of Glioblastoma Multiforme (GBM) and then imaged using MR at five time points. The final tumor sizes between mice varied dramatically. We model the growth of the tumor with a basic reaction-diffusion equation on a 3D finite-difference scheme and estimate parameters to generate best fitting tumors. We examine whether our optimized parameters lie within estimations from previous literature.

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MS25

Regulation of Glucagon Secretion and Glucagon Counterregulation in Type 1 Diabetes

In health, the pancreas secrets insulin and glucagon in a coordinated way to control glycaemia. In Type 1 diabetes (T1DM), lack of insulin is considered the primary abnormality. However, glucagon is also disordered. It is excessive postprandially, but insufficient in response to hypoglycemia. We propose an endocrine network model which unifies interactions between the major pancreatic peptides and blood glucose that can replicate the normal glucagon axis and explain its impairment in T1DM.

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MS25

Mathematical Modeling of Podocytes in Diabetic Kidney Disease

Diabetic kidney disease (DKD) is the primary cause for kidney failure and is a severe complication of diabetes. Damage to kidney cells called podocytes is a critical factor in the onset of DKD. We use a flux balance analysis approach to describe the biochemical reaction network kinetics and other factors that connect diabetic hyperglycemia to podocyte damage in DKD. Results are validated with published experimental data.

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MS25

A Mathematical Model of Type 2 Diabetes Driven by Insulin Hypersecretion

Type 2 diabetes is a disease that is conventionally assumed to arise from an inability of pancreatic beta-cells to produce sufficient insulin. In recent years, however, B. Corkey has revived the 'hypersecretion theory' of diabetes (Banting lecture, 2011) that postulates the disease arises from over-secretion of insulin. I will describe a minimal mathematical model that places the hypersecretion theory on a firm footing which suggests that it is plausible diabetogenesis may occur through this route.

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MS25

Diverse Pathways to Type 2 Diabetes

The heterogeneity in pathways of pathogenesis in type 2 diabetes (T2D) challenges medical management of T2D patients, or better, its prevention. We have updated our beta-cell mass and function model to include daily glucose dynamics and the kinetics of insulin granule exocytosis, providing insight into the various patterns of progression. The model suggests that the pathway to T2D depends on whether insulin resistance is in the peripheral tissues or the liver.

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MS26

Control of Voluntary Immune Suppression in Transplant Recipients

We consider mechanistic mathematical models for the human immune response system in the presence of both transplanted organs and the eruption of opportunistic viruses under immune-suppression. The problem of appropriate control of the suppression levels in long term individual patient therapy is addressed.

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MS26

Systems Models and Data Assimilation in Cardiometabolic Drug Development

Quantitative systems pharmacology models guide the integration of quantitative knowledge in the context of drug discovery by linking disease physiology and pharmacotherapy. Though a promising platform to identify disease subtypes and assess individual response to therapy, such models are not amenable to classical methods of data fitting and assimilation, owing to their size and complexity. Here, novel approaches to systems model development, calibration, and validation will be discussed, with examples from cardiometabolic drug development.

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MS26

Improving Protein-Bound Uremic Toxins Removal: Model and Multi-Objective Optimization Based Displacer Profiling

Hemodialysis (HD) sustains life in millions of renal failure patients. Primary purpose of HD is to remove toxins and excess fluid. Protein-bound uremic toxins (PBUTs) are especially hard to remove. A reactive separation technique holds the promise for improved removal of PBUTs. In this work, a novel mathematical model describing PBUT dynamics within the patient and in the dialyzer is developed. Based on multi-objective optimization a personalized dialysis regimen to maximize PBUT removal is also determined.

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MS26

Parameter Estimation and Uncertainty Analysis of a Vascular Refilling Model Using Hematocrit Data in Hemodialysis Treatment

A two-compartment model has been developed to describe the short-term dynamics of vascular refilling during ultrafiltration in hemodialysis. Relevant physiological parameters are identified using continuous hematocrit measurements. These parameter estimates could provide information on the (patho)physiological status of hemodialysis patients. In order for this information to be used in clinical decision-making, a degree of certainty should be assessed. Classical Sensitivity Analysis is used to determine the asymptotic standard errors of the estimated parameters.

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MS27

Jamming and Glassy Behavior in Dense Biological Tissues

Cells must move through tissues in many important biological processes, including embryonic development, cancer metastasis, and wound healing. Often these tissues are dense and a cell's motion is strongly constrained by its neighbors, leading to glassy dynamics. Although there is a density-driven glass transition in particle-based models for active matter, these cannot explain liquid-to-solid transitions in confluent tissues, where there are no gaps between cells and the packing fraction remains fixed and equal to unity. I will demonstrate the existence of a new type of rigidity transition that occurs in confluent tissue monolayers at constant density. The onset of rigidity is governed by a model parameter that encodes single-cell properties such as cell-cell adhesion and cortical tension. I will also introduce a new model that simultaneously captures polarized cell motility and multicellular interactions in a confluent tissue and identify a glassy transition line that originates at the critical point of the rigidity transition. This work suggests an experimentally accessible structural order parameter that specifies the entire transition surface separating fluid tissues and solid tissues. Finally I will present my collaboration work with the Fredberg group (Harvard School of Public Health), where these predictions have been successfully tested in bronchial epithelial cells from asthma patients, explaining pathologies in lung epithelia.

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MS27

Model Cell-ECM Interactions in Cancer Invasion

Extracellular matrix (ECM), a fibrous material that forms a network in a tissue, significantly affects many aspects of cellular behavior, including cell movement and proliferation. Transgenic mouse tumor studies indicate that excess collagen, a major component of ECM, enhances tumor formation and invasiveness. Moreover, cell interactions with the collagen matrix result in aligned fibers that facilitate cell invasion. However, the underlying mechanisms are unclear since the properties of ECM are complex, with diverse topographies and mechanical properties depending on various biophysical parameters. We have developed a three-dimensional elastic computational fiber network model, and parameterized it with in vitro collagen experiments. Using this model, we simulate mechanical testing of fiber networks and examine the mechanical and structural changes of fiber networks upon local deformation. We have also developed a cell migration model and a biomechanical cell-ECM interaction model, as initial first steps toward a fully biomechanical cell-matrix interaction model for cell migration and tumor invasion. I will show that this type of model has the potential to help us better understand cancer invasion and point to new therapeutic approaches.

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MS27

Modeling Keratinocyte Wound Healing: Cell-Cell Adhesion Promotes Collective Migration

The migration of epithelial sheets of keratinocyte cells in vitro displays behavioral and biochemical similarities to the in vivo wound healing response of keratinocytes in animal model systems. Epidermal Growth Factor Receptor (EGFR) activation through ligand binding mediates the forward migration of cells into the wound. Previous mathematical modeling studies propose that physical cell-cell adhesions have a hindering effect on the migration of collectively migrating cell populations, however, biological literature suggests cell-cell adhesion can promote such migration in some cases. To investigate the role of cell-cell adhesion on keratinocyte sheet migration, we developed two nonlinear diffusion models that assume cell-cell adhesion either hinders or promotes migration. While both models can accurately predict the forward migration of the leading edge of migrating keratinocyte sheets, the latter model assuming cell-cell adhesion promotes migration is robust to changes in the leading edge definition, as opposed to the other model. Using RNAi for the protein alpha-catenin, which is critical for cell-cell adhesion, we experimentally validate that sheets of cells with robust cell-cell junctions are able to better maintain collective migration than sheets of cells defective for cell-cell adhesion. Our modeling and experimental data suggest a positive role of cell-cell adhesion on sustained re-epithelialization of wounds.

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MS27

A Multiphase Complex-Fluids Model for Collective Cell Motions on Patterned Substrate

The collective motion of multicellular systems (a group of cells) on a substrate is a result of intercellular and intracellular dynamics coupled with the strong cell substrate interaction at different time and length scales. In this talk, a new multiphase complex fluids model will be presented to study this dynamics. The effects of microstructures of individual cells (cell membrane, cell cortex, actin polymerization/depolymerization) on the collective dynamics will be investigated. The cell substrate interaction and its role in directing cell motions will be studied, as well.

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MS28

Swimming in Complex Fluids: Experiments with Model Organisms

Many microorganisms (e.g. bacteria, algae, sperm cells) evolve and move in fluids that contain (bio)-polymers and/or solids. Examples include human cervical mucus, intestinal fluid, wet soil, and tissues. These so-called complex fluids often exhibit non-Newtonian rheological behavior due to the non-trivial interaction between the fluid microstructure and the applied stresses. In this talk, we will show that the material properties of such complex fluids can strongly affect the motility behavior of microorganisms such as the nematode C. elegans ($L \sim 1$ mm) and the algae C. reinhardtii ($L \sim 10$ μm). Fluids with a rage of material properties (viscosity behavior, elasticity) and structures (polymer networks) are used. Results show that fluid elasticity, for example, can significantly affect the swimming kinematics (beating frequency, bending curvature) of microorganisms beating cilia produces less curvature and C. elegans traveling wave speed decreases as elasticity increases. We also find that in some cases the addition of polymers to liquids can increase the organisms swimming speed (C. reinhardtii) while in other cases it can hinder self-propulsion (C. elegans). These results demonstrate the intimate link between swimming kinematics and fluid rheology, and that one can control the spreading and motility of microorganisms by tuning fluid properties.

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MS28

Oscillations in Active, Viscoelastic, Filament-Motor Biological Systems

Many biological organelles include thin elastic filamentous structures interacting with molecular motors and embedded in a noisy, complex fluid medium. Two examples of this are motility assays probing filaments interacting with molecular motors and the structurally ordered eukaryotic flagellum moving in a fluid. These composite active, soft assemblies demonstrate an amazing range of experimentally realized time periodic patterns such as rotating coils (assays) and graceful clock-like traveling waves (flagella). We propose a continuum theory that explains the onset of these instabilities, tracks critical points and allows for characterization of emergent non-linear solutions. The role of external viscoelasticity and intrinsic passive elasticity in stabilizing or disrupting these solutions are discussed.

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MS28

A Numerical Study on Flagellar Kinematics in Different Fluid Rheologies

It is observed in experiments that as the fluid rheology is changed, Chlamydomonas reinhardtii exhibits changes in both flagellar kinematics and the swimming speed. To understand this phenomenon, we develop a computational model of the swimmer, using flagellar strokes fit from experimental data. We discover that stroke patterns are the dominant factor for changing swimming speeds, and stroke patterns observed in viscoelastic fluids generate much lower stress at the cost of lower swimming speed.

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MS28

Flexibility and Waveform Analysis for Flagellar Motility in Viscoelastic Fluids

Biological micro-swimmers have soft bodies that respond to the external environment. Experiments have shown that flexible swimmers respond to fluid elasticity with stroke changes that enhance swimming. The mechanisms behind this fluid-body elasticity speed-up are not understood. We use asymptotic analysis of shape changes for flexible bodies driven by prescribed body moments to understand how fluid elasticity influences body kinematics, and we will analyze how these shape changes affect swimming speed.

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MS29

Mathematical Modeling and Computational Methods for the Tumor Microenvironment

The tumor microenvironment, which includes processes at the molecular, cellular and tissue scales, has become an important focus of study in recent years. One feature of the tumor microenvironment is generation of high acidity in response to low oxygen concentration (hypoxia). Hypoxia and acidosis promote metastasis, invasion and mutation. Although there have been many studies of the tumor microenvironment, most are based on PDEs where the cells are represented as a continuum or on discrete agent-based methods. Here, we describe a hybrid/cells-based model for the emergence of ductal carcinoma in situ (DCIS) and the transition to invasive ductal carcinoma (IDC) both in vivo and in vitro microfluidic devices. We present preliminary results for the microenvironment using simplified models of metabolism as well as the cellular response and production of diffusible growth factors such as TGF-beta. In this model, the cells are represented as discrete entities in which the fluid mechanical component is represented in an immersed boundary framework, the transport of ions and proteins by an immersed interface methods, coupled with systems of ODE's for the intracellular processes.

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MS29

Incorporating Cellular Substructure into Reaction-Diffusion Models

High resolution images of cells demonstrate the highly heterogeneous nature of both the nuclear and cytosolic spaces. We are interested in understanding how this complex environment might influence the dynamics of cellular processes. To investigate this question we have worked to develop particle-based stochastic reaction-diffusion methods that can track the spatial transport and reaction of individual molecules within domains derived from imaging data. As motivation, I will first describe some recent modeling work in which we have investigated how explicitly accounting for cellular organelles influences the time for a signal to propagate across the cytosol of cells. I will then introduce the convergent reaction-diffusion master equation (CRDME), a lattice particle-based stochastic reaction-diffusion model we are developing to allow the study of chemical pathways within such complex geometries. The CRDME is similar in spirit to the popular reaction-diffusion master equation (RDME) model. It allows for the reuse of the many extensions of the RDME developed to facilitate modeling within biologically realistic domains, while eliminating one of the major challenges in using the RDME model.

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MS29

Modeling Polymorphic Transformation of Bacterial Flagella

We present a fluid-structure interaction model of a single helical flagellum capable of polymorphic transformations. Bacteria cells swim forward by spinning its flagellar filaments counterclockwise, during which each flagellum takes a left-handed helical shape. To change course, several flagella will reverse rotation and spin clockwise changing the chirality of their helical form. Simulations of a single flagellum shows the transition from left- to right-handed form as the motor reverses which is similar to experimental observations.

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MS29

Mathematical Models of Telomere Length Regulation

Telomeres are repetitive noncoding DNA sequences that cap both ends of linear chromosomes. When a cell divides telomere length shortens, which can limit the number of times that a cell can divide. Cells with a large proliferation potential have mechanism to offset this telomere shortening. In this talk we will examine mathematical models that explore how telomere length is regulated in mammals and in certain species of yeast.

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MS30

Phase-Field Free Energy and Boundary Force for Molecular Solvation

We discuss a phase-filed variational model for the solvation of charged molecules with implicit solvent. The solvation free-energy functional of all phase fields consists of the surface energy, solute excluded volume and solute-solvent van der Waals dispersion energy, and electrostatic free energy. The last part is defined through the electrostatic potential governed by the Poisson-Boltzmann equation in which the dielectric coefficient is defined through a phase field. We prove Gamma- convergence of the phase field free-energy functional to its sharp-interface limit. We also define the dielectric boundary force for any phase field as the negative first variation of the free-energy functional, and prove the convergence of such force to the corresponding sharp-interface limit.

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MS30

Domain Dynamics of Lipid Vesicle Membranes

In lipid membranes, cholesterol combines with saturated lipids form energetically stable domains which are surrounded by unsaturated lipids. These domains coarsen with time, and the presence of external fluid flow or electric fields will impact the lipid domain growth rate. We numerically model this phenomenon with a surface Cahn-Hilliard-Cook equation using a combined level set/closet point method scheme. Quantitative measures of lipid domain growth and migration will be obtained and compared to experimental results.

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MS30

Calculating Energy Barriers and Activation States for Steps of Fusion

usion between biological membranes is a widespread cellular process, responsible for events as varied as secretion of neurotransmitters and fertilization of egg by sperm. Molecularly, fusion is the merger of two lipid bilayer membranes,and this merger proceeds through several key intermediates states. But the transition energy barriers that separate these intermediates have not been determined. Using the string method, we calculate a least energy pathway and the activation states between intermediates for the entire fusion process. The bilayer energetics are based on a modified Helfrich Hamiltonian that accounts for long range in-teractions between bilayers, and a novel field theoretic treatment of hydrophobic potentials. Through the energetic analysis, we conclude that lipid demixing is required for the transition from a stalk to a hemifusion diaphragm, and that complete fusion is possible provided pore formation is initiated while the diaphragm is small. The calculations provide a movie of individual lipid deformations, as the membrane geometry and topology evolve over time.

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MS30

Turning Phenomenon in a Physical Model of Cell Migration

In this talk, we present a comprehensive quantitative understanding of cell migration by reducing a complex dynamics of our previous work to a minimal model for the study of cell turning phenomenon. Numerical computations reveal how these factors conspire to control the turning instability in the cell migration process, and the corresponding phase diagrams for the minimal model and bifurcation analysis are presented.

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MS31

Computational Modeling of Early Brain Morphogenesis

During early development, the chick brain undergoes a combination of rightward torsion and ventral bending. This deformation is one of the earliest organ-level symmetry-breaking events in development. Previous evidence suggests that bending is caused by differential growth but our recent study shows that this torsion results from physical forces and is related to the asymmetric development of the heart. Here we develop a computational model that incorporates growth to interpret this unusual morphogenesis phenomenon.

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MS31

Modeling Growth of Residually Stressed Biological Tissue Within An Eulerian Framework

This talk gives a brief overview of an approach to modeling growth and remodeling of soft biological tissue within the context of an Eulerian framework of finite elasticity. The model accounts for the evolution of residual stress and is applied to an arterial wall subjected to chronic hypertension.

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MS31

Morphological Stability Analysis of An Elastic Tumor-Host Interface

The ability of tumors to metastasize is preceded by the presence of morphological instabilities, such as chains or fingers of cancerous cells that invade the host environment. In an effort to understand the role the tumor-host stiffness, we model the interface as an elastic membrane. Linear stability analysis using a Stokes model suggests bending rigidity is the most influential parameter and increased bending rigidity versus mitosis rate contributes to a more stable morphological behavior.

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MS31

A Viscoelastic Model of Blood Capillary Growth

This work studies a fundamental problem in blood capillary growth: how ell proliferation or death induces the stress response and the capillary extension or regression. The mathematical model treats the cell density as the growth pressure eliciting a viscoelastic response from the cells, which again induces extension or regression of the capillary. Numerical simulations demonstrate this model can reproduce angiogenesis experiments under everal biological conditions including blood vessel extension without proliferation and blood vessel regression.

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MS32

Effects of Temporal Noise versus Spatial Stochastic Distribution on Cardiac Focal Activity

Self-organization of interconnected elements is important for the development of cardiac biological pacemakers. Biological pacemakers are heterogeneous network of cells with some of the cells exhibiting spontaneous activation. Global spontaneous behavior has been shown to be dependent on stochastic distribution of pacemaker cells while noise-dependent acceleration and deceleration of activity can be found at the level of individual cells. The presentation will focus on how these two factors can interact to influence spatial-temporal spontaneous stability.

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MS32

Reconstructing 3D Reentrant Cardiac Electrical Wave Dynamics Using Data Assimilation

We present an approach for recovering the three-dimensional dynamics of reentrant waves in the heart by applying data-assimilation techniques to combine dual-surface observations with numerical model predictions. We use an ensemble Kalman filter method that is common in weather forecasting and evaluate the performance of the system using synthetic observations generated by the model. We present results from both a discordant alternans state in one spatial dimension and for scroll waves in three dimensions.

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MS32

Electrocardiac Defibrillation Simulations Using Sharp Boundary Method

Turbulence (fibrillation) in electrocardiac signal as a leading cause of death is commonly treated with a defibrillation electrical shock. We have developed a sharp boundary numerical method for defibrillation simulation. We study the role of electrical currents accumulating on the walls of blood vessels following a defibrillation electrical shock and at other locations, called virtual electrodes, in disrupting the filament which is a driving source of fibrillation.

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MS32

Estimation of Dynamical Variables in a Cardiac Myocyte Model

Cellular dynamical variables, such as ionic concentrations and gating states, play an important role in the formation of cardiac arrhythmias. Since these quantities can be difficult to measure, a Kalman filtering approach was tested on a myocyte model, and it was shown that cellular variables can be reconstructed based on simulated measurements of membrane potential. The observability of the system was characterized under a range of conditions.

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MS33

Collective Behavior in Systems with Active Sensing

Animal groups often serve as inspiration for mathematical models of collective behavior. Among such groups, bat swarms stand out as a unique system due to their use of biosonar, or echolocation, for sensing. Inspired by these animals, we model multi-agent systems with active sensing, which relies on a generated signal that can be intercepted by peers. To inform and validate these models, we analyze information transfer between wild bats flying together using model-free dynamical systems approaches.

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MS33

A Coupled Reaction-Diffusion Model for Gang Territorial Development

I will begin by providing an overview of the talks in this minisymposium. I will then introduce a lattice-based interacting particle model for gang territorial development motivated by graffiti deposition. In this model, there are two gangs who each deposit graffiti for their own gang. Each gang member performs a biased random walk to preferentially avoid the graffiti of the other gang. I will show numerical simulations of the agent-based model and describe the phase transition which occurs as the model's parameters are varied. I will then outline the formal derivation of the limiting system of coupled reaction-diffusion equations for the graffiti and gang member densities and discuss the properties of the system.

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MS33

Swarm Robotic Control Strategies Inspired by Biological Collective Behaviors

We address the problem of controlling robotic swarms that, like natural swarms, only have access to local information that is randomly encountered in the course of exploration.

We use stochastic and deterministic models from chemical kinetics and fluid dynamics to describe robots' roles, task transitions, spatiotemporal distributions, and manipulation dynamics at both the individual and population levels. In this talk, I describe our work on swarm control strategies for mapping, coverage, and ant-inspired collective transport.

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MS34

Linear Invariants for F81 and Other Evolutionary Models

The reconstruction of phylogenetic trees from molecular data relies on modelling site substitutions by a Markov process, or a mixture of such processes. In general, allowing mixed processes can result in different tree topologies becoming indistinguishable from the data, even for infinitely long sequences. However, when the underlying Markov process supports linear phylogenetic invariants, then if these are sufficiently informative, the identifiability of the tree topology can be restored. We investigate a class of processes that support linear invariants, the 'equal input model', once the stationary distribution is fixed. This model generalizes the 'Felsenstein 1981' model from four states to an arbitrary number of states (finite or infinite). We describe the structure and dimension of the vector space of phylogenetic mixtures (and the complementary space of linear invariants) for any fixed phylogenetic tree (and for all trees –the so called 'model invariants'), on any number of leaves.

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MS34

A Bayesian Approach to Inferring Rates of Selfing and Locus-Specific Mutation

We introduce a Bayesian method for estimating the selfing rate and locus-specific mutations rates. We extend the coalescent to accommodate selfing, and derive likelihood expressions for genotype data under the infinite alleles model. Mutation rates follow a Dirichlet Process Prior to pool information across loci. We additionally infer the number of generations since the most recent out-crossing event for each sampled individual. Our MCMC sampler can incorporate non-genotype data to infer additional parameters.

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MS34

Topological Algebras in Bacterial Genome Rearrangements

The inversion process in bacteria arises through the same biological process as knotting, and yet their modelling has always been approached with totally disjoint toolkits. I report on our progress towards a unified topological and algebraic framework employing so-called 'coloured link diagrams', where the sequential and topological aspects of site-specific recombinase and topoisomerase mechanisms occurring in the simplification pathways of bacterial DNA replication are simultaneously tracked.

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MS35

The Effect of Quasi-Steady-State Reductions in the Analysis of Biophysical Models

Many mathematical models of biological systems possess multiple timescales. A common first step in the analysis of such models is the elimination of one or more of the fastest variables via quasi-steady-state reduction (QSSR). A separation of timescales is not always sufficient to determine whether the application of QSSR yields a simplified model that has the same qualitative behaviour as the original model. For example, oscillatory solutions can be removed or dramatically changed by QSSR. We discuss effects of QSSR on well-known examples and present some general results for the persistence of Hopf bifurcations and the stability of slow manifolds.

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MS35

Finding Canards with the Zero Derivative Principle

Canards are solutions which stay close to repelling slow manifolds in multiscale dynamical systems. They play a major role in mixed-mode oscillations in neuroscience models. Canards are associated with the breakdown of Fenichel theory for slow manifolds. The zero derivative principle is a simple way of approximating slow Fenichel manifolds. We show that, surprisingly, it can be used to identify canards and canard explosions, even if the method is not expected to work here.

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MS35

Interacting Oscillation Mechanisms in Three-Time-Scale Systems

Oscillations in slow-fast systems can arise from slow passage through fast subsystem Hopf bifurcations or solutions tunnelling through twisted slow manifolds due to folded singularities. We examine the interaction of these oscillation mechanisms in the three-time-scale context, associated for example with neuronal bursting, where they naturally coexist. Analysis of a higher-codimension singularity, from which the Hopf and folded singularity unfold, elucidates properties of the local oscillatory behavior such as frequency, bifurcation delay, and rotation number.

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MS35

Generic Torus Canards and A Novel Class of Elliptic Bursting Rhythms

Torus canards are solutions of slow/fast systems that alternate between attracting and repelling manifolds of limit cycles of the fast subsystem. In neural applications, they mediate the transition from spiking to bursting. In this work, we formally prove that the average of a torus canard is a folded singularity canard. We use our theoretical framework to identify and analyze a novel class of elliptic bursting rhythms in a model for intracellular calcium dynamics.

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MS36

Symmetries Constrain Dynamics in a Family of Balanced Neural Networks

We examine a family of balanced excitatory/inhibitory firing-rate neural networks, and find that this system may be described as a perturbation from a system with non-trivial symmetries. We analyze the symmetric system using the tools of equivariant bifurcation theory and demonstrate that symmetry-implied structures remain evident in the perturbed system. In comparison, spectral characteristics of the network coupling matrix are relatively uninformative about the behavior of the perturbed system.

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MS36

Building a Theory of Subsampled Networks from the Bottom Up

Unraveling how unobserved or pooled neural signals influence the behavior of recorded neurons is a major challenge in neuroscience. Effective neural connections inferred from data are vulnerable to the influence of hidden neurons, and we lack a theory that relates these connections to the ground-truth connectivity. In this talk I will present a mathematical framework we are building to predict how inferred interactions between observed neurons or pooled signals are shaped by unobserved network properties.

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MS36

Learning and Evidence Accumulation in Changing Environments

To navigate a constantly changing world, we intuitively use the most recent and pertinent information. For instance, when planning a route between home and work we use recent reports of accidents and weather. We discount older information, as our environment is in constant flux: The clouds threatening rain last night may have dissipated, and an accident reported an hour ago has likely been cleared. How to make decisions in face of uncertainty and impermanence is a question that recurs in a variety of fields, and is of fundamental importance in neuroscience. Here, we explore this problem in a general setting where an observer evaluates multiple options based on a series of noisy observations. We assume that the best option changes in time. The optimal strategy is therefore to sequentially update the probability of each alternative, weighting recent evidence more strongly. This problem becomes even more challenging when the variability of the environment is unknown. A plausible neural implementation of an optimal observer in a changing environment shows that, in contrast to previous models, neural populations representing alternate choices are coupled through excitation.

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MS36

Spiking and Oscillatory Dynamics in the Frontoparietal Attention Network during Sustained Attention in the Ferret

Sustained attention requires the coordination of neural activity across multiple areas in the frontoparietal network. Previous work has demonstrated that during attention, activity in these brain regions is coordinated by neural oscillations in specific frequency bands. However, the underlying mechanisms of coordinated activity in these brain areas in terms of organization of spiking activity have remained poorly understood. We present experimental results which elucidate the frequency-specific organization of spiking activity and information transfer within and between prefrontal cortex and posterior parietal cortex of the frontoparietal attention network.

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MS37

Detecting Protein Coevolutionary Signals in the Absence of Persistent Structural Order

Intrinsically disordered proteins are characterized by regions in amino-acid sequence that have transient three-dimensional structure, providing many functional advantages through conformational flexibility. However, this also presents many challenges to existing methods in comparative analysis that require a reliable multiple sequence alignment to understand the relationships between known proteins. We show how co-evolutionary signals might be deconvolved, and discuss the implications for the role of primary structure in protein interactions based on these results.

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MS37

Phenotypic Buffering and Adaptation

In 1942, Waddington proposed that the adaptation of organisms to their environment in the course of evolution is enhanced by reducing the phenotyic effects of small changes in genotype. Because this idea is strongly counterintuitive, others have suggested the opposite. We investigate this problem numerically by modeling genotype, phenotype, mutation, and population dynamics in a changing environment. We report on how the rate of adaptation changes in response to the level of phenotypic buffering.

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MS37

Modeling Evolution at Multiple Scales in the Context of Host-Pathogen Coevolution

There is a long history of using gene regulatory network (GRN) models to understand the evolution of robustness to genetic and environmental perturbations, usually assuming stabilizing selection. We are exploring such models in the context of coevolution. We started with a host-parasite GRN coevolution model and have now developed our models further to include realistic epidemiology (SIS model) and pathogen-host receptor interactions in the context of host-pathogen coevolution.

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MS38

Diversity and Selection in Adaptive Immune Repertoires

Recognition ofpathogens relies on the diversity of immune receptorproteins. Recent experiments that sequence the entire immunecell repertoires provide a new opportunity for quantitative insight into naturally occurring diversityand how it is generated. The generation process is implemented via a series ofstochastic molecular events involving gene choices and random nucleotide insertions between, and deletions from, genes. I will describe a fast algorithm for quantifying the origins of diversityin these sequence and characterize selection in the somatic evolutionary process that leads to the observed receptor diversity.

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MS38

Computational Modelling of Adaptive Immune Responses to Influenza Vaccination

Abstract not available.

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MS38

Computational Methods for Repertoire Diversity Estimate

B and T cell receptor frequencies often follow heavy tailed distributions. We developed a power-law based estimator of allele and haplotype diversities (the total number of different receptors in this case, but the same can be applied to any allele) that accommodates heavy tails using the concepts of regular variation and occupancy distributions. Application of our methods to multiple T and B cell receptors repertoire yields an estimate of 1.e6-1.e8 different clones per compartment.

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MS38

Exploring Antibody Recognition by Comparing Mathematical Models with High-Throughput Antibody Binding Data

Antibodies are proteins used by the immune system to recognize molecular structures. However, the antibody mixture contained in blood is of unknown complexity. To gain insights into the recognition capabilities of antibodies, we formulated mathematical models of antibody binding. Based on mechanistic and statistical models, we discuss the features necessary for robust and specific recognition, and compare our hypothesis with available high-throuput antibody binding data.

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MS39

Evolutionary Dynamics of Cancer and its Response to Treatment

Cancer is the result of a stochastic evolutionary process characterized by the accumulation of mutations that are responsible for tumor growth, immune escape, and drug resistance, as well as mutations with no effect on the phenotype. Stochastic modeling can be used to describe the dynamics of tumor cell populations and obtain insights into the hidden evolutionary processes leading to cancer. I will present recent approaches that use branching process models of cancer evolution to quantify intra-tumor heterogeneity and the development of drug resistance, and their implications for interpretation of cancer sequencing data and the design of optimal treatment strategies.

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MS39

How a Tumors Phenotypic Distribution Can Guide Treatment Strategy

Tumors may be made of very homogenous or heterogeneous populations of cells. A targeted anticancer drug applied to a homogenous tumor might lead to easy eradication, but with heterogeneous populations it may lead to the selection of resistant phenotypes and ultimate disease recurrence. We explore how to use tumor characteristics such as size and phenotypic composition and variance to inform treatment strategy choices, which will best control a specific tumor.

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MS39

Tumor Heterogeneity and its Implications in Drug Resistance

Resistance to chemotherapy is one of the major causes of the failure of cancer treatment. Furthermore, recent experimental evidence suggests that drug resistance is a complex biological phenomena, with many competing aspects interacting nonlinearly. In this talk, we study models of tumor heterogeneity and drug resistance. Specifically, we discuss a general framework for modeling resistance, as well as specific model of cell-cycle resistance.

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MS39

Optimizing Oncolytic Virotherapy in Combination with Immunostimulation

Oncolytic viruses (OVs) have been engineered to treat cancer by selectively replicating inside of and lysing tumor cells. However, the efficacy of this process is limited. To combat these limitations, new OVs are being designed to mediate tumor cell release of cytokines and co-stimulatory molecules that attract cytotoxic T cells to target tumor cells, thus increasing the tumor-killing effects of OVs. Treatment efficacy can be further improved by combing OVs with dendritic cell (DC) injections. To investigate this combination mathematically, we built a model consisting of a system of ordinary differential equations and fit the model to the data provided from Huang *et al.* We then simulated varying doses of OV and DC injections to test a multitude of treatment strategies. In this talk, I will describe the model and report our results.

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MS40

Multiscale Modeling of Angiogenesis

Tumors induce the growth of new blood vessels from existing vasculature through angiogenesis. Using an agent-based approach, we model the behavior of individual endothelial cells during angiogenesis and determine collective behavior, in terms of partial differential equations (PDEs), using a Master equation framework. We find that multiple PDE models capture the same micro-scale mechanisms, and that PDEs cannot distinguish between certain types of micro-scale behavior. This may impact drug development strategies based on PDE models.

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MS40

Kinetic Monte Carlo Simulations of Multicellular Aggregate Self-Assembly in Biofabrication

We present a three-dimensional lattice model to study self-assembly and fusion of multicellular aggregate systems by using kinetic Monte Carlo (KMC) simulations. This model is developed to describe and predict the time evolution of postprinting morphological structure formation during tissue or organ maturation in a novel biofabrication process (or technology) known as bioprinting. In this new technology, live multicellular aggregates as bio-ink are used to make tissue or organ constructs via the layer-by-layer deposition technique in biocompatible hydrogels; the printed bio-constructs embedded in the hydrogels are then placed in bioreactors to undergo the self-assembly process to form the desired functional tissue or organ products. Here we implement our model with an efficient KMC algorithm to simulate the making of a set of tissues/organs in several designer's geometries like a ring, a sheet and a tube, which can involve a large number of cells and various other support materials like agarose constructs etc. We also study the process of cell sorting/migration within the cellular aggregates formed by multiple types of cells with different adhesivities.

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MS40

A Hydrodynamic Model of Cell Cytokinesis Driven by Actomyosin Contractile Ring

Cell Mitosis is a fundamental process in eukaryotic cell reproduction, during which parent cells nucleus first dissembles leading to DNA and chromosome replication, then chromosomes migrate to new locations within the parent cell to form offspring nuclei which triggers cytokinesis leading to the formation of two offspring cells eventually. In this presentation, we develop a full 3D multiphase hydrodynamic model to study the fundamental mitotic mechanism in cytokinesis, the final stage of mitosis. The model describes the cortical layer, a cytoplasmic layer next to the cell membrane rich in F-actins and myosins, as an active liquid crystal system and integrate the extra cellular matrix material and the nucleus into a multiphase complex fluid mixture. With the novel active matter model built in the system, our 3D simulations show very good qualitative agreement with the experimental obtained images. The hydrodynamical model together with the GPU-based numerical solver provides an effective tool for studying cell mitosis theoretically and computationally.

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MS40

Hydrodynamic Theories for Pattern Formation in Clusters of Stem Cells and Differentiated Cells

In many tissues, such as skin or intestinal epithelial, stem cells lie in periodic local areas. In the areas, stem cells divide and differentiate without migration, whereas the differentiated cells migrate out of the local areas actively. Even though the previous model for stem cell patterns considered all the hydrodynamical couplings allowed by symmetry, it is still based on assumption that there was no spontaneous polarization in the homogeneous state. To extend the model, we derive a hydrodynamic model based on the Generalized Onsager Principle. In this model, the spontaneous polarity states, birth and death of cells, self-propelled motion of differentiated cells and ATP hydrolysis are all accounted for. Linear stability analysis is conducted to reveal the long-wave instability inherent in the neighborhood of the constant steady states. The spatial patterns due to instability are observed in numerical experiments. Especially, new spatial patterns with spontaneous polarity are observed. Comparison with previous models will be presented in this talk.

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MS41

Wonders of Bacterial Motility

Escherichia coli swims by rotating long, thin, helical filaments that arise at different points on the cell surface. Each filament is driven at its base by a reversible rotary motor. Another Gram-negative bacterium, Flavobacterium johnsoniae, glides across solid surfaces without the aide of flagella, by moving surface adhesins. These appear to be propelled by rotary motors, but how does one go from rotation to translation? Do cells have treads, as in a snowmobile?

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MS41

Effects of Shear on Bacterial Motility in Porous Media Flows

Swimming cells play integral roles in bioremediation in porous soils and infections in human tissues. Understanding the physical mechanisms underlying cell transport in heterogeneous fluid environments is key to controlling these processes. Using microfluidic devices, we precisely prescribe the microstructure and flow within model porous media. We show that such confined flows generate significant heterogeneity in the spatial distribution of motile bacteria, as well as suppress the transport coefficients of active cells in porous media.

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MS41

Role of Flagellar Bending Stiffness on Sperm Motility

The axoneme of flagella and cilia are composed of microtubules that provide flexural rigidity. In this study, we use a mechanical model of an idealized sperm flagellum in a viscous, incompressible fluid. The mechanical forces are due to passive stiffness properties and active bending moments are based on a preferred curvature. The model is calibrated to experimental results and we examine the effects of the elastic properties of the flagellum on swimming patterns.

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MS41

Marine Bacteria Exploit a Flagellar Buckling Instability for Reorientation and Chemotaxis

Marine bacteria have a single flagellum and swim at high speeds in a recently discovered 'run-reverse-flick' pattern. The 'flicks' are large and fast angular reorientations, which are induced by a buckling instability of the 100-nm long 'hook' at the base of the flagellum, in a striking microscale example of failure turned into function. This talk will discuss the flick and how it relates to the motility pattern and chemotactic search strategy of marine bacteria.

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MS42

Abrupt Transitions to High Frequency Firing Caused by Recurrent Excitation in Neuronal Networks

We study neuronal networks in which there is "recurrent excitation", that is, cells excite each other. Recurrent excitation can lead to discontinuities in the dependence of frequency on parameters, with abrupt transitions from low-frequency firing or quiescence to high-freqency "runaway" firing. We study firing frequency as a function of the strengths of external and recurrent excitation, and show how discontinuities result from the interaction of fast recurrent excitation with slower feedback inhibition.

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MS42

From a Network of 10,000 Neurons to a Smartphone App with 125,000 Users: Linking Scales in Biological Rhythms

I will describe mathematical models of networks of neurons and chemical reactions within neurons that generate daily (circadian) timekeeping. The key question is how GABA is used in the timekeeping network of 10,000 neurons in the suprachiasmatic nucleus send multiple simultaneous signals to coordinate timekeeping and track the seasons. This work will be linked to a recent smartphone app we developed and used to globally track and study sleep.

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MS42

Modeling Type 2 Diabetes Pathogenesis

In the standard model for type 2 diabetes, obesity causes insulin resistance, requiring supra-normal insulin levels to control glucose. If the pancreatic beta cells cannot compensate, blood glucose rises. However, in pre-diabetes insulin rises before glucose. This has led to an alternate model: high insulin secretion causes high glucose by triggering insulin resistance. We show that the standard model accounts for the observed dynamics of glucose and insulin and clarifies important clinical issues.

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MS42

Calcium Dynamics: The Interaction of Theory and Experiment

In almost every cell type, oscillations in the concentration of intracellular calcium are crucial for controlling a myriad of cellular processes ranging from secretion, to contraction, to gene expression. Their physiological importance and dynamic complexity make them an ideal subject of study by both experimentalists and theoreticians, and thus the field of calcium signalling has been a fruitful interdisciplinary research area for over 30 years. I shall talk about a range of questions in calcium signalling, showing how close interaction between experimentalists and modellers can lead to insights that would be difficult to attain by either separately, and how advances in one discipline can contribute to advances in the other. As it happens, the very first person to talk to me about calcium signalling was Charlie Peskin, which is yet another example of how he has educated and inspired multiple generations of mathematical biologists around the world. So, if I feel brave, I will also talk briefly about how Charlie took an ignorant young mathematician from New Zealand and did his best to turn a sow's ear into a ... well, maybe a cheap plastic supermarket bag. We all stand on the shoulders of giants, and Charlie is one of my own particular giants.

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MS43

Differential Geometry Based Multiscale Solvation Models

Abstract not available.

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MS43

Solvation Free Energy Decomposition Using the 3D-RISM Theory of Molecular Solvation

The decomposition of solvation free energies (SFEs) into polar/non-polar, energy/entropy and spatial components can yield deep insights into biological processes but is often computationally challenging. Here we present an overview of the 3D reference interaction site model (3D-RISM) theory of molecular solvation and its ability to rapidly compute these SFE components. We demonstrate the accuracy of 3D-RISM on several large data sets of charged and neutral small molecules in aqueous and non-polar solvents, where we achieve the same level of accuracy as all-atom molecular simulation. These are important milestones in developing robust, accurate and efficient methods for understanding fundamental biology and applications like drug discovery and design.

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MS43

Adaptive Boundaries and Transferable Potentials in Multi-Resolution Simulations

Biomolecular simulations require a compromise between forcefield resolution and computational efficiency. Methods that combine multiple levels of resolution promise to extend the ability of simulations to handle bigger systems and more complex processes. We have developed an explicit/continuum solvent model that is able to reproduce the effects of explicit solvation with only a fraction of the molecules that would otherwise be required. We are extending this approach as a general multi-resolution model where both solvent and other, more complex, molecules change representation as they move across the boundaries of the explicit and continuum domains. This model includes: (1) boundary methods that accurately reproduce thermodynamic and kinetic properties in the explicit region exactly, within statistical error, as if they were taken from large, fully explicit simulations; (2) adaptive boundaries that alter the size of the high resolution region in response to an evolving molecular environment; and (3) a grand canonical control of molecular components, relaxing the density of chemical species as the simulation progresses. Our current work is aimed at transferability to new systems and arbitrary geometries. Overcoming this challenge will be important to making these multi-resolution models ready to be used out of the box for a range of problems in biophysics.

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MS43

Modeling and Computation of Molecular Solvation

In this talk, I will give a briefly review of a few implicit solvent models for solvation analysis. The second-order accurate method for implicit solvent models will be presented. Hybrid physical and statistical models will be introduced for the blind prediction of solvation free energies. Finally, I will discuss a knowledge based model for blind solvation prediction.

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MS44

Mathematical Modeling of Human Pregnant Cervix

The human cervix is a significant mechanical valve to keep the fetus inside the uterus during pregnancy for a full term birth. The cervix volume change and its internal fiber remodeling are two important factors contributing to the cervical mechanical effect during pregnancy. We combine the two factors in the modeling, and understand how together the fetus weight, intrauterine pressure and cervical surrounding structure form the mechanical distribution of the cervix.

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MS44

A Biochemical and Mechanical Model of Injury-Induced Intimal Thickening

In this talk, we investigate an axisymmetric model of intimal thickening using hyperelasticity theory. Our model describes the growth of the arterial intima due to cell proliferation, which, in turn, is driven by the release of cytokines. We compare our model predictions to rabbit and rodent models of atherosclerosis and find that in order to achieve the growth rates reported in the experiments, growth must be mainly cytokine induced rather than stress induced.

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MS44

Modeling the Effects of Focal Adhesion Size and Distribution on Stress Fiber Activity and Cell Shape

We present a two-dimensional model and finite element simulations of a cell interacting with a deformable substrate through evolving focal adhesion (FA) complexes. Our aim is to understand how controlling the size of FAs, either via disassembly by microtubules or by ligand patterning, affects cellular responses. We compare the effects of two proposed models for controlling FA evolution on intracellular stresses, substrate displacement patterns, FA distribution, and cell shape for different substrate stiffnesses and ligand patterns.

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MS44

Modeling of Growth, Gene, and Protein Expression in Biofilms

Reporter gene, transcriptomic, and proteomic technologies have made it possible to measure gene and protein expression in microbial biofilms. How can differences in biofilm gene expression, both in comparison to planktonic cells and in space and time within the biofilm, be understood? Here we provide general theoretical framework for addressing this question. At the core of the model are reaction-diffusion equations that account for microscale concentration gradients within the biofilm. We will present the study of four specific cases including: Inducible GFP, Denitrification, Acid stress response, and Quorum sensing. Comparison between model simulations and experimental results will be given.

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MS45

A Catheter-Simulator Software Tool to Generate Electrograms of Any Multi-Polar Diagnostic Catheter from 2D and 3D Atrial Tissue

The simulation software allows users to place a multi-pole catheter on atrial endocardial surface and record simulated electrograms. In 2D, the catheter geometry is created using samples from equation of circle along the plane of surface. In 3D, the plane of principle curvature is determined using eigenvectors of catheter vertices, from where the normals are projected and registered to the surface using 3D geodesic distance. This tool provides a platform for performing customized cardiac experiments.

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MS45

Patient-Specific Fitting of Detailed and Simplified Models of Human Atrial Myocytes for Modeling Atrial Fibrillation

The Fenton-Karma and Koivumaki-Korhonen-Tavi models were fit to five sets of data obtained from patients with AF at invasive electrophysiological study. Each model was simultaneously fitted to the action potential morphology, action potential duration restitution, and the conduction velocity restitution curves. Parameter sets were obtained for each patient that accurately reproduced the data, but differed significantly from the original published values. The resulting spiral wave dynamics and stability in 2D domains is also shown.

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MS45

Credibility of Predictions of Computational Models of the Heart Given Validation Evidence

We will discuss methods for assessing the credibility of computational cardiac models, in particular focusing on determining how 'applicable' a model and its validation evidence are to a proposed 'context of use'. As with many computational models that have medical applications, with heart models 'direct validation'—comparison of model and experiment in identical conditions—is usually impossible, raising questions about credibility of predictions. We will demonstrate using cardiac examples a systematic approach for assessing credibility.

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MS45

New Approaches to Identify the Pivot Point of Rotor

Atrial fibrillation (AF) is the most common sustained cardiac arrhythmia and is a prognosis marker for stroke, heart failure and death. It is believed that stable electrical sources of cardiac excitation (rotors) can cause AF and therefore, the pivot points (core) of rotors are considered to be good ablation targets for AF termination. Here we propose and validate, using ex-vivo animal experiments, several techniques for accurate identification of the pivot points of rotors

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MS46

Models of Collective Dynamics with Complex Orientation Mechanisms

In this minisymposium, we will report on recent developments on self-propelled particle models with complex orientation mechanisms. The most simple and widely studied orientation mechanism involves polar orientation and follows from the seminal work of Vicsek and co-authors. The macroscopic dynamics of this model gives rise to the SOH model (self-organized hydrodynamics) which has been shown to exhibit many surprising and unusual behavior. However, other orientation mechanisms can be found in nature such as nematic alignment or alignment of the full body configuration. We will present microscopic and macroscopic versions of these dynamics and outline some applications to bacterial colonies and flocking.

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MS46

Lane Formation by Side-Stepping

In this talk we present a non-linear convection-diffusion model, which describes the evolution of two pedestrian groups walking in opposite direction. We start from a two-dimensional lattice based model and formally derive the corresponding limiting equations using Taylor expansion. We introduce an entropy functional, which allows us to obtain the necessary estimates to prove global existence of bounded weak solutions. Furthermore we illustrate the dynamics with various numerical simulations.

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MS46

A Boltzmann Mean Field Game Model for Knowledge Growth

In this talk we present a Boltzmann type mean field game model for knowledge growth, which was proposed by Lucas and Moll in 2013. The model consists of a coupled system of a Boltzmann type equation for the agent density and a Hamilton-Jacobi-Bellman equation for the optimal strategy. We study the analytic features of each equation separately and show local in time existence and uniqueness for the fully coupled system. Furthermore we focus on the construction and existence of special solutions, which relate to exponential growth in time - so called balanced growth path solutions. Finally we illustrate the behavior of solutions for the full system and the balanced growth path equations with numerical simulations.

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MS47

Split Scores on Phylogenetic Trees with Applica-

tions

From DNA sequence data collected from n taxa, we construct a 'split score' under the assumption that the aligned sequences have evolved under the general Markov model (GM) on an evolutionary tree. This split score, based on theoretical properties for the GM model on trees, can be computed efficiently from genomic scale data using the singular value decomposition. In this talk, we describe this split score and illustrate how it might be used to detect true splits in the evolutionary tree relating taxa, and shifts in the evolutionary process along a chromosome.

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MS47

Inequality-Based Gene Tree Invariants and Phylogenomic Species Tree Inference

Phylogenetic invariants, introduced in 1987 as polynomial equalities in probabilities of different nucleotide sequences under mutation models on trees, spurred the development of methods for phylogenetic inference using algebraic geometry and statistics. The concept of invariants was recently extended to include algebraic relations between probabilities of *gene trees*, or trees inferred using data from multiple loci in a collection of genomes (also known as phylogenomic data). We examine the promising consequences of focusing on inequalities as gene tree invariants (instead of equalities) and discuss difficulties that arise when using invariant-based approaches on real and simulated phylogenomic data.

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MS47

Displayed Trees Do Not Determine Distinguishability Under the Network Multispecies Coalescent

Recent work in estimating species relationships have included rooted networks to represent speciation and hybridization. Gene trees evolve within such networks. We show that there are cases in which two distinct networks can not be distinguished using only one genetic lineage per species but can be distinguished with more than one lineage per species. We also show that two networks that display the same trees can sometimes be distinguished with one lineage sampled per species.

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MS47

Invariant Measures and Unbiased Statistics for Phylogenetic Quartet Estimation

I will discuss recent work which uses representation theory to give a complete analysis of the transformation properties (both discrete and continuous) of phylogenetic invariants on quartet trees. This analysis leads to the development of least-squares measures of quartet fitness that are statistically unbiased and satisfy strong invariance properties under multinomial sampling. I will present specific results for the binary state space and discuss how the theory is full generalizable to a state space of any size. This is joint work with Amelia Taylor, Barbara Holland, and Peter Jarvis.

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MS48

Combining Global Parameter Sampling and Bifurcation Analysis to Study Electrical Activity in a Pituitary Cell Model

Pituitary corticotrophs have variable patterns of spontaneous electrical activity, including quiescence, spiking, and bursting oscillations. Stimulation by hormones CRH and AVP increases activity via several proposed mechanisms. We study spontaneous and stimulated activity in a corticotroph model by generating a wide variety of spontanous patterns through GPU-accelerated sampling of parameter space. We use direct numerical simulation and bifurcation analysis to understand how hormone-induced activity changes depend on the context of other model parameters.

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MS48

Averaging, Folded Singularities and Torus Canards: Investigating Transitions in a Neuronal Model

Bursting behavior in neurons plays a critical role in driving repetitive actions such as respiration and hormone release. However, neurons may exhibit other behavior such as quiescence or tonic spiking. In this talk, we examine a model of two synaptically coupled respiratory neurons from the pre-Bötzinger complex. We analyze the transitions between bursting and spiking behavior in the model using slow-fast decomposition and averaging methods, and elucidate the central role of folded singularities.

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MS48

Subthreshold Amplitude and Phase Resonance in Models of Quadratic Type: Nonlinear Effects Generated by the Interplay of Slow Resonant and Fast Amplifying Currents

We investigate the biophysical and dynamic mechanisms of generation of preferred amplitude and phase responses to oscillatory inputs (resonance and phasonance) in neuronal models featuring nonlinearities of parabolic type in the voltage nullcline. These models capture the interplay of the so-called resonant (e.g. hyperpolarization-activated) and amplifying (e.g., persistent sodium) currents in biophysically realistic parameter regimes. We determine how the nonlinear effects affect the response and their dependence on the participating explicit and effective time scales.

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MS48

A Study of the Synchronization Between Two Coupled Neuron Models Generating Mixed-Mode Oscillations

We analyze a 6D slow-fast system consisting of two coupled identical 3D oscillators formed by a FitzHugh-Nagumo system with an additional slow variable generating Mixed-Mode Oscillations. Such system has been built to account for the impact of slowly evolving intracellular calcium concentration upon the neuron electrical activity. We derive the global bifurcation diagram, focus on the synchronization properties of the oscillators and point out the role of MMOs in the birth of the different patterns.

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MS49

Uncovering Cellular Properties from Network Dynamics

Functionally equivalent neuronal circuits can generate similar activity patterns despite disparate intrinsic and synaptic properties. We use conductance-based models to investigate the role of descending inputs in regulating the output of a simple circuit comprised of two mutually inhibitory non-identical neurons. Can we uncover differences in circuit properties (intrinsic and synaptic) by examining circuit output to external stimuli? We consider the robustness of circuit output (e.g. half-center oscillating activity) in response to stimuli with different statistics, for pairs of circuits different properties. We discuss the robustness in the context of trade-offs between synaptic and intrinsic circuit properties, which has implications for neuromodulation and plasticity that can dynamically change these properties.

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MS49

Conflict Resolution by a Hippocampal Attractor Network

An attractor neural network is an influential theory describing how a network of hippocampal place cells may form a cognitive, spatial map of an environment. I examine the interactions among conflicting external inputs and internal dynamics of an attractor network of place cells. Analysis and numerical simulations reveal the network architecture under which spurious attractor states arise. Results are compared to electrophysiological data for which rats must resolve conflicting information from local and global cues.

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MS49

Stimulus-Induced Changes in Spiking Co-Variability in Two Populations

Recent simultaneous array recordings of the olfactory bulb and piriform cortex in rat show distinct spiking statistics depending on state (spontaneous or odor-evoked). Like other sensory systems, the firing rate increases with stimuli. However, the spike count correlation/co-variability changes in different ways depending on the population. We present some preliminary modeling work to better understand network attributes that explain the data. This will ultimately impact how signals are coded in these distinct areas.

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MS49

Metastability of Gene Networks

Metastable transitions are rare events, such as bistable switching, that occur under weak noise conditions, causing dramatic shifts in the expression of a gene. Within a gene circuit, one or more genes randomly switch between regulatory states, each having a different mRNA transcription rate. The circuit is self regulating when the proteins it produces affect the rate of switching between gene regulatory states. Under weak noise conditions, the deterministic forces are much stronger than fluctuations from gene switching and protein synthesis. A general tool used to describe metastability is the quasi stationary analysis (QSA). A large deviation principle is derived so that the QSA can explicitly account for random gene switching without using an adiabatic limit or diffusion approximation, which are unreliable and inaccurate for metastable events.This allows the existing asymptotic and numerical methods that have been developed for continuous Markov processes to be used to analyze the full model.

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MS51

Cancer Stem Cells, Hierarchically Organized Tumors and Estimating Treatment Outcomes Using Mathematical Modeling and Patient-Specific Tumor Burden

Many tumors are hierarchically organized and driven by a sub-population of tumor initiating cells (TICs), or cancer stem cells. TICs are uniquely capable of recapitulating the tumor and are implied to be highly resistant. Macroscopic patterns of tumor expansion and regression during treatment are tied to TIC dynamics. Until now, quantitative information about the fraction of TICs from macroscopic tumor burden trajectories could not be inferred. We generated a quantitative method based on a mathematical model that describes hierarchically organized tumor dynamics and patient-derived tumor burden. The method identifies two characteristic equilibrium TIC regimes during expansion and regression. We show that tumor expansion/regression curves can be leveraged to infer estimates of the TIC fraction in individual patients. Furthermore, our method is parameter-free; it solely requires knowledge of a patient's tumor burden over multiple time points to reveal microscopic properties of the malignancy. We demonstrate proof of concept in the case of chronic myeloid leukemia (CML): our model recapitulated the clinical history of the disease in two independent patient cohorts. Based on patient-specific treatment responses in CML, we predict that after one year of targeted treatment, the fraction of TICs increases 100-fold and continues to increase up to 1000-fold after five years of treatment.

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MS51

Limiting the Development of Anti-Cancer Drug Resistance in a Spatial Model of Micro-Metastases

Using a hybrid spatial model, we explore how chemoresistance in micrometastases depends on the drug dosing schedule. We separately consider weakly and strongly resistant populations that can acquire drug resistance, or can harbor pre-existing resistance. Simulations uncovered several intermittent protocols that eradicate strongly acquired micrometastases resistant to continuous therapy, and also eradicate weakly resistant micrometastases (acquired and pre-existing) more efficiently than continuous therapy. These protocols may represent more effective chemotherapy schedules to limit metastatic progression.

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MS51

Mathematical Modelling of Cancer Heterogeneity and Drug Resistance

Heterogeneity among cellular populations has recently been identified as a significantly important factor complicating and impeding treatment response in a number of solid tumors. This heterogeneity giving rise to diverse phenotypes may be explained by both the standard theory of clonal evolution or the cancer stem cell (CSC) hypothesis. According to the CSC theory, in addition to their self-renewal, CSCs can undergo symmetric or asymmetric "unidirectional" divisions to generate daughter cells with low tumorigenic potential (non-CSCs). However, growing evidence supports violation of unidirectionality for the traditional stem cell based tissue hierarchy, suggesting a new model in which a significant degree of plasticity exists between the non-CSC and CSC compartments. This talk will survey our mathematical approaches to investigate the CSC hypothesis and the dynamic phenotypic switching between these populations, as well as therapeutic implications.

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MS51

Mathematical Models of Cancer Vaccines: How to Get the Right Things to the Right Place at the Right Time

Mathematical models of cancer vaccines: how to get the right things to the right place at the right time. Abstract: We have developed mathematical models of cancer and the immune response that can be calibrated to individual patients in order to predict outcomes of cancer vaccines. These models can be used to answer clinically relevant questions, such as when and where to administer the vaccine, and how these answers vary between individuals. However, recent clinical trials have revealed new challenges. Laboratory research shows that the tumor environment is immunosuppressive, reducing the effectiveness of vaccines. Recently, immunologists have identified specific mechanisms by which the tumor cells can escape recognition by killer immune cells and new immunotherapies are being developed to block these mechanisms. In this talk, we describe an extension of previous models that includes these immuno-suppressant blockers in addition to immuno-stimulating vaccines. Optimisation techniques will be discussed that can be used to suggest treatment and targeted delivery strategies for these new combination immunotherapies.

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MS52

Mechanical Insights into the Adhesion Dynamics of Amoeboid Cells

Amoeboid migration requires cells to undergo large shape changes, and to apply highly coordinated mechanical forces on the environment by means of transient cell-matrix adhesions. Despite recent studies, the mechanisms of rapid shape changes and how they lead to migration are still unclear. We developed a computational model to study the interplay of cellular mechanics, cell-substrate interaction, and the resulting migration. This work shows that the motility coordination observed in *Dictyostelium discoideum* amoeba emerges from these main components: actin polymerization, cortical tension, and the mechanochemical response of adhesive bonds.

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MS52

Determining the Rheological Properties of Actin

Actin, which is involved in cell motility, ranges from $0.5 - 5mM$, intracellularly. Thus, the mechanics of motility depends upon actin biophysics at these high concentrations. Most work in this field sites Schmidt, Ziemann and Sackmann, who addressed actin incompressibility in 1996. To improve upon their work, we have revisited this problem using modern experimental technology and numerical mathematics. We describe our process, present the results and outline the implications for cell motility models.

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MS52

Mathematical Modeling of Actin Regulation in Invasive Carcinoma

Expressions of actin regulators are altered in metastatic carcinomas. I will discuss research in collaboration with John Condeelis on modeling actin growth in lamellipodia and invadopodia, two distinct motility structures in metastatic cells. In lamellipodia, cofilin severs old F-actin generating new barbed ends upon stimulation, but the role of cofilin in invadopodia may only be crucial at later time points. I will compare actin dynamics and the temporal regulations of cofilin in these two structures.

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MS52

3D Model of Cytokinetic Contractile Ring Assembly: Node-Mediated and "Backup" Pathways

Cytokinetic ring assembly in fission yeast involves condensation of actin filaments and myosin motors bound to the cell membrane through cortical nodes. It is unclear how rings form in mutant cells that fail to recruit myosin to nodes and how ring formation is rescued after node clump formation (backup pathway). A 3D computational model based on Bidone et al. (Biophys. J, 2014) provides a mechanistic explanation of ring assembly in mutants by assuming actin-dependent binding of diffusive myosin to the cortex.

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MS53

Impacts of the Competition for Phytoplankton Organic Matter in Marine Bacteria

Microscale interactions between bacteria and phytoplankton underpin ocean biogeochemistry, but it remains unclear how consequences of these interactions propagate to the larger ecosystem. Making use of a detailed experimental characterization of a lysing diatom with chemotactic bacteria, we model the competition for dissolved organic matter between heterotrophs and oligotrophs. In the context of diatom blooms in coastal ecosystems, we find that chemotaxis drives initial bacterial population succession and has important implications in nutrient partitioning.

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MS53

Intersections Between Chemical Signaling, Microbial Interactions, and the Ocean's Biological Carbon Pump

Microbial controls on a number of important biogeochemical fluxes of carbon and nutrients in the ocean have eluded explanation, including the sequestration of carbon via the biological pump. Our work is elucidating the long-ago recognized, but largely unexplored potential for chemical signals to control microbial interactions, and, thus, the biological pump. This work has been catalyzed by major technological advances in mass spectrometry, which now allow the analysis of chemical signals at *in situ* concentrations.

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MS53

Swimming in Confined Microgeometries

We examine the behavior of microswimmers confined to Hele-Shaw type geometries, and show surprising results in their collective dynamics. For example, we show hydrodynamically-triggered transitions from turbulent-like swimming to aggregation and clustering. When subject to circular confinement in the Hele-Shaw plane, the swimmers could exhibit global orientational order into vortex-like structures. The collective dynamics is even more interesting in narrow rectangular channels, where we observe the emergence of compression and expansion density shock waves.

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MS53

Global Estimates of Bacterial Attachment to Particles Sinking in the Ocean

Bacteria colonize organic particles sinking from the sunlit surface to deeper depths in the ocean. The particles are oases of food for bacteria, which solubilize and consume organic carbon from the particles. The rates at which bacteria colonize particles determine whether abundances of bacteria on particles are sufficient for group behaviors. Using numerical models, we predict where bacterial group behavior on particles is likely to occur in the global ocean.

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MS54

A Lubricated Immersed Boundary Method in Two Dimensions

We describe an immersed boundary method that uses elements of lubrication theory to resolve thin fluid layers between immersed boundaries. Such methods are useful for simulating the passage of deformable elastic capsules through narrow constrictions, such as the transit of red blood cells through the narrow slits in the spleen and the intracellular trafficking of vesicles into dendritic spines. Making use of simple two-dimensional flows with known exact solutions, we will show convergence results illustrating the increased accuracy in comparison to the standard immersed boundary method.

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MS54

Two Extensions of the Immersed Boundary Method and Their Applications

The immersed boundary (IB) method is a generally useful computational method for problems in which elastic materials interact with a viscous incompressible fluid. In this talk, we introduce two extensions of the IB method. The first one, which is called the penalty IB method, is introduced to take into account both the inertial and gravitational effects of the elastic materials with mass. The example problems include vortex induced vibration, 3D parachute, Rayleigh Taylor instability and its dynamic stabilization. The second extension is to deal with the case in which the immersed boundary is a porous material though which the surrounding fluid passes. As the application examples of the present method, we will show the simulation results on 2D parachute, 2D and 3D dry foam dynamics.

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MS54

Vesicle Electrohydrodynamics Simulations by Coupling Immersed Boundary and Immersed Interface Methods

In this talk, we introduce a coupling immersed boundary (IB) and immersed interface method (IIM) to simulate the electrodeformation and electrohydrodynamics of a vesicle in Navier-Stokes leaky dielectric fluids under a DC electric field. The vesicle membrane is modeled as an inextensible elastic interface with an electric capacitance and an electric conductance. Within the leaky dielectric framework and the piecewise constant electric properties in each fluid, the electric stress can be treated as an interfacial force so that both the membrane electric and mechanical forces can be formulated in a unified immersed boundary method. The electric potential and transmembrane potential are solved simultaneously via an efficient immersed interface method. The fluid variables in Navier-Stokes equations are solved using a projection method on a staggered MAC grid while the electric potential is solved at the cell center. A series of numerical tests have been carefully conducted to illustrate the accuracy and applicability of the present method to simulate vesicle electrohydrodynamics.

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MS54

From IB to IIM, from Solution to Gradient Computations, From Algorithm to Convergence Analysis Convergence Analysis

The Immersed Interface Method (IIM) was motivated by Peskin's Immersed Boundary (IB) method for better accuracy and to deal with discontinuous coefficients. Recently, we have proved that the IB method is inconsistent but first order accurate in the L^∞ norm while the IIM is second order accurate both for the solution and the gradient by Beale/Layton for Poisson interface problems.
In this talk, the emphasis is to explain recent development of IIM and augmented IIM not only for second order accurate solution but also for second order accurate gradient for interface problems with variable but discontinuous coefficients. The key of the new method is to introduce the jump in the normal derivative of the solution as augmented

variable and re-write the interface problem as a Laplacian of the solution with lower order terms near the interface. Thus we can get jump relations for send order derivatives using the augmented variable and lower order terms. The idea should be applicable for boundary value problems as well. An upwind type discretization is used for the finite difference discretization near or on the interface so that the discrete coefficient matrix is an M-matrix. We also provide the proof of the convergence of the proposed method. Numerical examples with non-trivial and general interfaces are also provided.

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MS55

Extracting Nonlocal Models from Experimental Measurements and Detailed Atomistic Simulation

Atomistically detailed molecular dynamics (MD) simulations have proven fruitful in understanding biological processes at a fundamental level. Here we discuss the use of MD simulations to understand the dielectric function of the water around a protein. The dielectric function can then be used as the basis for a multiscale continuum model that offers the speed of classical PoissonBoltzmann models while adding important structural details such as charge layering.

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MS55

Accounting for Water's Finite Size Using the Mean-Spherical Approximation as a Modified Dielectric Boundary Condition

A multiscale hydration-shell boundary condition (HSBC) is proposed that can successfully reproduce Gibbs solvation free energy for a Born ion from the mean-spherical approximation (MSA) model. In contradiction of traditional dielectric models, this model (HSBC/MSA) also can reproduce the solvation entropy correctly. It only depends on the normal electric field at the dielectric boundary and it is independent of the ion radius. This feature enables us to utilize it for complex molecules such as proteins.

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MS55

Effects of Conformational Dynamics and Macromolecular Crowding on Biomolecular Electrostatic Design Efforts

Electrostatic interactions between biomolecules can be sensitive to conformational dynamics and their environment. In particular, the characteristics of a molecules optimal binding partner could depend strongly on these factors. Through a continuum electrostatics framework, we analyze the contributions of different structural and chemical moieties toward binding interactions and calculate hypothetical molecular charge distributions that maximize electrostatic affinity. By integrating these analyses with molecular dynamics simulations and models for cellular crowding, we probe how the optimal electrostatic properties of a molecule change. Applying these techniques to proteinprotein and drugtarget systems can provide insights into both natural molecular recognition and drug design.

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MS56

Open Source Agent-Based Simulations of Large 3-D Multicellular Tumor-Stromal Systems

We will present open source software we are developing for data-driven investigations of multicellular systems, including BioFVM (finite volume method for biological problems), which simulates diffusion of many substrates in 3D tissues; PhysiCell (physics-based cell simulator), which simulates systems of 10^5 to 10^6 off-lattice cells in 3D tissues with microenvironment-dependent phenotypes; parameter identification tools; and MultiCellDS (multicellular data standard) for data sharing. These parallelized codes run on desktop workstations. Further details at MathCancer.org and MultiCellDS.org.

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MS56

Agent-Based Modeling of Cyanobacteria Nitrogen Metabolism and Ecology

Anabaena populations are complex systems, including multiple nitrogen assimilation pathways and cell types (photosynthesizing vegetative cells and nitrogen fixing heterocysts). We developed a new agent-based model of Anabaena, based on our current understanding of its biology and a large database of empirical observations. This model reproduces the major observed patterns and helps to interpret experimental data. We used it to predict the response to nutrient reduction scenarios aimed at controlling eutrophication of a lake.

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MS56

Agent-Based Simulation of Viscoelastic Microbial Aggregate Growth in an Arbitrary Flow Field

In population balance modeling literature, the mathematical forms used for growth rates are derived for an idealized spherical aggregate and assume that all aggregates of size x are identical. However, the microbial aggregates are highly fractal structures and thus aggregate structure heterogeneity must be included in the modeling of the growth rates. We use an off-lattice individual-based model to simulate the growth of virtual microbial clusters and derive growth rates from this simulations.

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MS57

Filament Tension of Meandering Scroll Waves

The dynamics of spiral waves in systems that yield circular tip trajectories is relatively well understood, and their response to small perturbations can be predicted using response function theory. The long-term behaviour of 3D scroll waves is determined by the sign of the filament tension, which determines whether the filament length increases or decreases over time. Here, I present an extension of response function theory to meandering spiral waves, and discuss how filament tension generalises to filaments with meandering core.

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MS57

Chaotic Transients in Physiologically Realistic Models of Cardiac Tissue

Simple reaction-diffusion models of excitable media are known to exhibit transient spiral wave turbulencea chaotic state that reaches an asymptotic, non-chaotic state in finite time. We extend these results by investigating the properties of transient spiral chaos (i.e. fibrillation) in physiologically realistic models of cardiac tissue. In particular, we seek to understand how the turbulent lifetime scales with domain size and how it is affected by spiral wave meandering instability.

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MS57

Structural Features of Quasi-Stationary Multi-Spiral States in a Simple Model of Atrial Fibrillation

The transition from single-spiral to multi-spiral configurations can be understood as a connection along the unstable manifold of the single-spiral state. Additionally, weak interactions between spiral cores suggests that important properties of quasi-stationary multi-spiral solutions may be understood from single-spiral solutions. In this talk I describe the shape and slow evolution of multi-spiral states in terms of their constituent parts, i.e., single spirals, their breakups, and mergers.

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MS57

Modification of Scroll Wave Filaments When Electric Fields Are Applied to the Heart

The effects electric field pulses have on action potential scroll wave filaments differ considerably from those induced by conventional localized electrical stimuli. In this talk, I will review the generic effects produced by these pulses, and then describe important modifications to these effects produced by the proximity of system boundaries and by spiral wave meandering. These studies will help us to understand the basic bioelectric response of heart tissue to newly proposed low-energy defibrillation protocols.

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MS58

Scaling Laws and Asymptotics in Single Particle Modeling

The characterization of anomalous diffusion calls for scale-free analysis. In this talk, we will address the issue of scaling laws arising in single particle experiments. First, following Didier and Zhang (2016), we will look at the asymptotic distribution of the diffusion estimator widely used in the biophysical literature, the sample mean square displacement. Second, we will discuss the bivariate analysis of particle paths according to the wavelet eigenstructure approach, as recently proposed in Abry and Didier (2016).

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MS58

Diffusion and Transient Binding with a Non-Linear Tether

In living cellls, Brownian forces play a dominant role in the movement of small and not so small particles, such as vesicles, organelles, etc. However, proteins and other macromolecules bind to one another, altering the underlying Brownian dynamics. In this talk, classical approaches in the biophysical literature to time series which switch between bound and unbound states will be presented, and an alternative approach using stochastic expectation-maximization algorithm (EM) combined with particle filters will be proposed along with extensions for non-quadratic potentials when the particle is bound. As an example system, molecular motors, such as kinesin, switch between weakly and strongly bound states, as well as directed transport. I will discuss the analysis of such a system along with the ramifications for multi-motor-cargo complexes found in living cells and studied in vitro.

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MS58

Linear Regression Analysis on FRAP and FCS and its Application to Anomalous Diffusion Processes on Cell Membranes

Diffusion of proteins and other biomolecules in lipid membranes is one of the most fundamental biological processes and underlies almost all the aspects of cellular signaling. Therefore, accurate quantification of the diffusion in membranes is a key factor to understand biochemistry and biophysics of cellular signaling processes. Due to complex cellular environments, diffusion in lipid membranes often shows a nonlinear relation in time, e.g. anomalous diffusion and is often described as a time dependent diffusion coefficient, $D(t)$. Currently, a handful of methods are available to measure $D(t)$ including Fluorescence Recovery after Photobleaching (FRAP), Fluorescence Correlation Spectroscopy (FCS), Single Particle Tracking (SPT), and Nuclear Magnetic Resonance (NMR). Nevertheless, current models and measurements of anomalous diffusion using these methods have major limitations. Here, we develop a novel theoretical/computational methodology for easily accessible technologies, such as FRAP or FCS to determine $D(t)$ without a single power law assumption and to apply the methodology to measure $D(t)$ of model proteins and lipid probes.

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MS59

Dynamics of Hearing: The Active Ear

As a biological detector, the vertebrate ear exhibits a remarkable variety of dynamical behavior that provides fertile ground for mathematical study. The goal of this talk is two-fold. First, general background on the ear will be provided to set a basis for the the talks comprising the symposium. Second, we will explore a remarkable aspect of hearing: The ear not only responds to sound, but generates and coherently emits it as well. These sounds, called otoacoustic emissions (OAEs), provide crucial insight into inner ear function. To explore the biophysical processes possibly giving rise to spontaneous emissions (SOAEs), we will focus on a theoretical framework based upon coupled active nonlinear oscillators. To help constrain such an SOAE model, we also report recent empirical data that characterize SOAE dynamics and their perturbations due to external transient stimuli.

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MS59

Consequences of Organ of Corti Micro-Mechanics

In the mammalian cochlea, small vibrations of the sensory epithelium are amplified due to the active mechanical feedback of the outer hair cells. High frequency sounds encoded in the basal cochlea are amplified more than low frequency sounds. This location-dependent amplification has been a characteristic used to validate theoretical models. However, different models rely on different mechanisms to achieve the location-dependent amplification. For example, some studies have considered greater active feedback force toward the base, but other studies explored alternative mechanisms such as tonotopically varying electrical properties of the outer hair cells. We have developed a computational model of the cochlea featuring continuum mechanics-based organ of Corti mechanics, and realistic physiological properties of the outer hair cell. Using the computational model, we show that the organ of Corti micro-mechanics can explain the location-dependent amplification. Specifically, the timing of outer hair cell force generation with regard to its deformation changes depending the location. Our results show that this timing is determined by the passive mechanics. To support the conclusion, we present: 1) the power flux along the cochlear length, 2) the spatial pattern of outer hair cell power generation, 3) the effect of local inhibition of outer hair cell force, and 4) the effect of the RC time constant of outer hair cell membrane.

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MS59

Bifurcations of a Noisy Biological Oscillator are Associated with Function

Hair bundles actively transduce mechanical stimuli into electrical signals in the auditory, vestibular, and lateral-line systems of vertebrates. Theory predicts that a bundle's function is dictated by whether it operates near particular types of bifurcation. We confirmed these predictions by employing a feedback system to change the operating point of individual hair bundles. We identified two kinds of bifurcation, despite the presence of substantial environmental noise, associated with three distinct types of signal detector.

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MS59

The 3D Wkb Method Applied for the Calculation of Cochlear Viscous Fluid Loss and Outer-Hair Cell Power Generation

Abstract not available.

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MS60

Facets and Relaxations of the Balanced Minimal Evolution Polytope

The balanced minimal evolution (BME) method of creating phylogenetic trees can be formulated as a linear programming problem, minimizing an inner product over the vertices of the BME polytope. We report on the project of describing the facets of this polytope. We classify and identify the combinatorial structure and geometry (facet inequalities) of all the facets in dimensions up to 5, and classify several types of facets in all dimensions. We want a subset of facets that provide efficient relaxations of the BME polytope. We note the fact that all 654,729,075 phylogenetic trees on 12 taxa are recovered in the 54 dimensional polytope defined by our list of facet inequalities.

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MS60

Statistically-Consistent K-Mer Methods for Phylogenetic Tree Reconstruction

Frequencies of k-mers in sequences are sometimes used as a basis for inferring phylogenetic trees without first obtaining a multiple sequence alignment. We show that a standard approach of using the squared-Euclidean distance between k-mer vectors to approximate a tree metric can be statistically inconsistent. To remedy this, we derive model-based distance corrections for orthologous sequences without gaps, which lead to consistent tree inference. The identifiability of model parameters from k-mer frequencies is also studied. Finally, we report simulations showing the corrected distance out-performs many other k-mer methods, even when sequences are generated with an insertion and deletion process. These results have implications for multiple sequence alignment as well, since k-mer methods are usually the first step in constructing a guide tree for such algorithms. Joint work with Elizabeth Allman and John Rhodes. Do not include references or citations separately at the end of the abstract. Instead, all citations must be in text in the general form [Authorname, Title, etc]

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MS60

Stochastic Safety Radius on NJ and BME Methods for Small Trees

A distance-based method to reconstruct a phylogenetic tree with n leaves takes a distance matrix, $n \times n$ symmetric matrix with 0s in the diagonal as its input and it reconstructs a tree with n leaves using tools in combinatorics. A safety radius is a radius from a tree metric, a distance matrix realizing a true tree where the input distance matrices all lie within, in order to satisfy a precise combinatorial condition under which the distance-based method is guaranteed to return a correct tree. A stochastic safety radius is a safety radius under which the distance-based method is guaranteed to return a correct tree within a certain probability. In this talk we investigated stochastic safety radii for the neighbor-joining (NJ) method and balanced minimal evolution (BME) method for n = 5.

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MS60

Convexity in Tree Spaces

We study the geometry of metrics and convexity structures on the space of phylogenetic trees, here realized as the tropical linear space of all ultrametrics. The CAT(0)-metric of Billera-Holmes-Vogtman arises from the theory of orthant spaces. While its geodesics can be computed by the Owen-Provan algorithm, geodesic triangles are complicated and can have arbitrarily high dimension. Tropical convexity and the tropical metric are better behaved, as they exhibit properties that are desirable for geometric statistics.

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MS61

Reduced Dimensional Map for the Circadian Regulation of Human Sleep

The disruption to sleep that occurs when sleep is initiated at different circadian phases is a well-known side effect of jet lag. For a biophysical model of sleep-wake regulation for human sleep, we have constructed a map that tracks the day-by-day evolution of the circadian phases of sleep onset when sleep and circadian cycles are not entrained. The piecewise continuous structure of the map reflects discontinuous modulation of sleep patterns due to circadian phase and rapid eye movement sleep behavior.

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MS61

Developing Mathematical Models for Circadian and Sleep-Dependent Modulation of Pain

Numerous experimental studies have identified interrelationships between modulation of pain by sleep behavior and circadian rhythms. To investigate these interactions, we use two different mathematical modeling frameworks: First, we construct a modified two-process model to make predictions for pain sensitivity under different scenarios of sleep disruption. Second, we consider the average firing rate of neuron populations in the dorsal horn and construct a novel biophysical model for pain that mimics empirical observations.

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MS61

Modeling the Effects of Temperature on Sleep Patterns

Experimental work and prior models suggest changes in ambient temperature can affect sleep patterns in humans. We have designed a mathematical model describing numerous features of the human sleep–wake cycle and aspects of REM–non-REM dynamics. The model simulates temperature changes detected by neurons in the POAH that, in turn, affect the REM–non-REM cycles during sleep through a state-dependent homeostatic process. This model serves to better understand the role temperature plays in abnormal sleep behavior.

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MS61

Patterns of Sleep-Wake Behaviour: From Maps to Naps

Even very simple models of sleep-wake regulation exhibit a rich dynamical behaviour, including daily patterns with a single sleep episode (monophasic sleep), or multiple sleep episodes (polyphasic sleep). We show how transitions between different patterns occur via grazing bifurcations. Such bifurcations could explain the change from polyphasic to monophasic sleep during the first five years of human life and how different sleep patterns observed in different species could result from the same underlying biological mechanisms.

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MS62

Compressive Sensing Reconstruction of Feed-Forward Connectivity in Pulse-Coupled Nonlinear Neuronal Networks

Utilizing the sparsity ubiquitous in neuronal network connectivity, we develop a framework for efficiently reconstructing feed-forward connections in nonlinear neuronal networks through their output activities. Using only a small ensemble of random inputs, we solve this inverse problem through compressive sensing theory based on a linear structure intrinsic to the nonlinear network dynamics. The accuracy of the reconstruction is verified by the fact that complex inputs can be well recovered using the reconstructed network connectivity.

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MS62

Rich Club Dynamics in Networks of Cortical Neurons

We used a 512 electrode array to record spiking activity at the millisecond scale from networks containing several hundred cortical neurons. Functional connectivity revealed a rich-club structure, where hub neurons were more likely than chance to be connected to each other. Using models fitted to the data, we found that the rich club had profound effects on spike synchrony, population coupling and the generation of long avalanches.

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MS62

Feedback Through Graph Motifs Relates Structure and Function in Complex Networks.

How does the connectivity of a network system combine with the property of individual components to determine its collective function? We approach this question by relating the internal network feedback to the statistical prevalence of connectivity motifs, a set of local network statistics. This provides a reduced order model of the network input-output dynamics. We show how this enables robust, yet tunable, functionality such as extending the time constant with which networks remember past signals.

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MS62

The Impact of Complex Network Structures on Seizure Activity Induced by Depolarization Block

Cessation of inhibitory activity due to depolarization block often precedes epileptiform activity suggesting its role in seizure initiation. Previous computational studies investigated pathological network dynamics arising from excitatory-inhibitory networks when inhibitory neurons are prone to depolarization block. In this talk, we discuss how complex network structures may affect the dynamical landscape created by depolarization block.

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MS63

Rabies Persistence in Vampire Bats: Immunity, Pathogenesis, and Immigration

Abstract not available.

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MS63

Emerging Disease Dynamics in a Model Coupling Within-Host and Between-Host Systems

Abstract not available.

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MS63

Epidemiological Signatures of Imperfect Vaccines in Structured Populations

Abstract not available.

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MS63

Inferring Cross-Immunity in Multi-Pathogen Systems

Abstract not available.

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MS64

Exploring Model and Clinical Trial Uncertainty Using Virtual Populations

The parameters of a physiological model are rarely fully identifiable from the available data. The resulting uncertainty in parameters may be sampled to create alternative

parameterizations of the model, sometimes termed virtual patients. Here we introduce a novel technique to efficiently generate virtual patients and construct a virtual population that matches observed data. This approach improves confidence in model predictions by mitigating the risk that spurious virtual patients become over-represented in virtual populations.

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MS64

Mathematical Modeling to Aid Enterprise Wide Decision Making for Drug Discovery, Manufacturing, and Marketing

Applied mathematics has been a well accepted medium to answer scientific questions and aid drug discovery. Over the last decade this capability has widened its role to also solve manufacturing, marketing, and business decision making problems for pharmaceutical companies. In this talk, we will outline the strategic importance of mathematical modeling with a few examples and measurable benefits.

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MS64

Stuff I Wish I Had Paid Better Attention to in Grad School: Lessons Learned from Mathematical Modeling in Cancer Drug Development

From Descartes rule of signs, to phase portraits of dynamical systems, to existence/uniqueness proofs, mathematical modeling in oncology drug development is replete with high school, college, and graduate level applied math problems. Several quantitative systems pharmacology applications will be presented, for example: characterizing bivalent activation artifacts of an antagonist antibody; dynamical systems analysis and Fokker-Planck models of antibody-dependent cell-mediated cytotoxicity (ADCC) in immuno-oncology; predicting long-term tumor relapse from initial response and ex vivo assay data.

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MS64

A Brief Introduction to Some Mathematics of Data Privacy

The expression or paradox of the *irresistible force against an immovable object* may seem to be embodied in the life sciences as the irresistible argument to broadly share important clinical trial data against the immovable privacy guarantees to patients within these trials. Recently, mathematicians have been exploring how to quantify privacy and create anonymous or synthetic databases. We discuss this quantification and provide some examples and analysis showing there is safety/privacy in numbers (of patients) and sampling accuracy in those same numbers.

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MS65

Force Generation and Contraction of Random Actomyosin Rings

We investigate computationally the self-organization and contraction of an actomyosin ring that is completely disorganized initially. To this end, we formulate a detailed agent-based model for a 1D chain of cross-linked actin filaments forming a closed ring interspersed with myosin-II motor proteins. The result of our numerical experiments is that in order to contract, 1) actin filaments in the ring have to turn over, 2) myosin motors have to be processive, and 3) filaments have to be sufficiently crosslinked. Moreover, the model demonstrates that with time, a pattern formation takes place in the ring attenuating the contraction. Finally we derive a continuum model as a short filament limit of the agent based model. The model features highly nontrivial pattern formation and traveling wave solutions and explains the aggregation of actin and myosin predicted by the microscopic model.

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MS65

The Role of Cytoplasmic Rheology in Blebbing Dynamics

Blebs are pressure-driven protrusions that play an important role in cell migration, particularly in 3D environments. A bleb is initiated when the cytoskeleton detaches from the cell membrane, resulting in the pressure-driven flow of cytosol towards the area of detachment and local expansion of the cell membrane. Recent experiments involving blebbing cells have led to conflicting hypotheses regarding intracellular pressure dynamics. We develop a dynamic computational model of the cell to simulate these experiments, and show that complex rheology of cytoplasm is essential to explain experimental observations.

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MS65

A Computational Model of YAP/TAZ Mechano-Sensing Mechanism

In cell proliferation and differentiation, YAP/TAZ serves as an important mechanical checkpoint regulating cellular fate, with the mechanism of integrating mechanical signals elusive. Thus, a computational model of YAP/TAZ activity integrating cell-matrix adhesion, signal transmission and cytoskeleton dynamics can predict molecular/mechanical interventions in silico. This integrated molecular model explains the synergistic effect between the mechano-sensing and the Hippo pathway. We provide this platform to investigate molecular/mechanical regulators on development, tissue engineering and tumor progression.

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MS65

A Role of Functional Heterogeneity of Endothelial Cells in Stabilization of Vascular Tube Formations

Cerebral Cavernous Malformations (CCMs) develop in about 0.5 percent of the population worldwide. This disease is caused by mutations in one of three genes ccm-1, -2, or -3 that lead to enlarged leaky blood vessels. People with CCM experience seizures, paralysis, cerebral hemorrhage, and loss of hearing or vision. To understand the defects that lead to loss of proper vascular tube formation in CCM patients, we developed a novel computational image analysis technique to quantify the dynamics of individual cells and parametrize a multi-cell model for the collective behavior of endothelia cells during tube formation. Our multi-cell model takes into account interactions of the cells with the extracellular matrix and each other through the extension and retraction of protrusions. The model also allows for cell movement and changes in shape in response to forces exerted by neighboring cells. Our simulations not only reproduced experimentally observed patterns of tube formation in wild type and CCM knockdown cells, but also captured differences between the behavior of CCM1 and CCM3 deficient cells, providing mechanistic insight into the distinct roles of these proteins. Furthermore, the model predicts that splitting of the initially identical cells into functionally distinct groups is essential for the formation of mechanically stable cell patterns and that this process is disrupted in CCM.

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MS66

Simulating a Post-Fragmentation Probability Density Function for Microbial Flocculation

We present a model to compute the force on the surface of a fluid ellipsoidal droplet in simple shear flow, constructed from existing models for the evolution in shape and orientation of a fluid droplet and for the force density on the surface of a solid ellipsoidal particle. We apply this model in a simulation of microbial floc fragmentation to generate a post-fragmentation probability density function, and compare the results to a previous simulation in which the flocs are treated as non-deforming.

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MS66

Ferromagnetic and Antiferromagnetic Order in Bacterial Vortex Lattices

Despite their inherent non-equilibrium nature, living systems can self-organize in highly ordered collective states that share striking similarities with the thermodynamic equilibrium phases of conventional condensed matter and fluid systems. Through microfluidic experiments and mathematical modelling, we demonstrate that lattices of hydrodynamically coupled bacterial vortices can spontaneously organize into distinct phases of ferro- and antiferromagnetic order. The emergence of opposing order regimes is linked to geometry-induced edge currents, reminiscent of those in quantum systems.

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MS66

Biodegradation of Dispersed Crude Oil Droplets by Diffusive Encounters with Non-Motile Microbes in Marine Environments

Hydrocarbon droplets are dispersed throughout the water column and persist in the environment until they are physically encountered by oil degrading microorganisms. Currently, there is a lack in understanding the direct link between droplet size and specific oil biodegradation rates in marine systems. Here, we present a mechanistic encounter-consumption model founded on microscale laboratory observations that predicts the oil degradation time by non-motile bacteria as a function of oil concentration, droplet diameter, and bacterial growth.

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MS66

A Numerical Study of Fluid Transport by Migrating Zooplankton Aggregations

Diel vertical migrations of zooplankton aggregations have been hypothesized to play an important role in local nutrient transport and ocean dynamics. Recent efforts have been made both experimentally and numerically to better understand the impact of these naturally occurring biological processes. By implementing solutions to the Stokes equations, numerical models have successfully captured the time-averaged far-field flow generated by self-propelled swimmers. However, discrepancies between numerical fluid transport estimates and in-situ field measurements of individual swimming jellyfish suggest the need to include near-field effects in order to correctly assess the impact of biogenic mixing in oceanic processes. Furthermore, a recent experimental study has shown that additional mechanisms responsible for enhanced transport are triggered during collective motion, a complex feature that has not yet been included in numerical models. In this talk, the inherent difficulty of modeling the unsteady flow of active swimmers while including near-field effects is bypassed by integrating experimental velocity data of zooplankton onto a numerical model. Fluid transport is investigated by tracking a sheet of artificial fluid particles during vertical motion of zooplankton organisms. Collective effects are addressed by studying different swimmer configurations within a migrating aggregation from the gathered data for a single swimming animal.

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MS67

Stochastic Immersed Boundary Methods for Fluid-Structure Interactions Subject to Thermal Fluctuations

Stochastic immersed boundary methods provide a promising approach for mesoscopic modelling and simulation of elastic structures that interact with a fluid when subject to thermal fluctuations. This allows for capturing simultaneously such effects as the Brownian motion of spatially extended mechanical structures as well as their hydrodynamic coupling and responses to external flows. These fluctuating hydrodynamics approaches handle the hydrodynamic equations directly allowing for spatially adaptive discretizations or domains having complicated geometries. However, this presents the challenge of numerically approximating a set of stiff stochastic partial differential equations (SPDEs) having non-classical solutions (distributions). We introduce stochastic discretization procedures based on ideas from statistical mechanics and Ito calculus. We show how efficient stochastic computational methods can be developed for viable fluctuating hydrodynamic simulations. We demonstrate these methods in the context of applications including the simulation of transport within microfluidic devices, particle dynamics within curved manifolds representing lipid bilayer membranes, and the rheological responses of soft materials. We also plan to survey current challenges and opportunities for fluctuating hydrodynamic approaches.

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MS67

Error Estimates for Finite Difference Methods Applied to Navier-Stokes Flow with Interfaces

Computations of Navier-Stokes flow with a moving boundary have been done using finite differences on a regular grid with the immersed interface method. It is observed that, with viscosity not small, the error in velocity can be about $O(h^2)$ near the interface even if the truncation error is $O(h)$ there. We will present error estimates which explain how such accuracy can be achieved. We will first describe maximum norm estimates for finite difference versions of the Poisson equation and diffusion equation with a gain of regularity. We will then describe the application to the Navier-Stokes equations of fluid flow in a prototype problem, neglecting errors in the interface location. The analytical methods are generally discrete analogues of standard methods for partial differential equations.

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MS67

Computing Insect Flight

Abstract not available.

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MS67

Modeling and Simulation of an Elastic Sheet with a Non-Newtonian Fluid

Motivated by fluid-structure-interaction (FSI) phenomena in life sciences (e.g., erythrocytes moving in flowing blood), we consider a simple FSI model problem — interaction of an elastic sheet (fixed at the midline) with a non-Newtonian fluid in three dimensions. The non-Newtonian flow is modelled by the lattice Boltzmann method. The deformable structure and the FSI interaction are handled by the immersed boundary (IB) method. Effects of fluid property, Reynolds number, and sheet bending rigidity are investigated.

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MS68

Comparison of PB Solvers Using CG and DG Methods

In this talk, the methods of CG and DG used in this work are introduced first, they have both been realized on nodal based FEM. Then the method for solving the PBE is introduced. They are both based on the time dependent PBE. Time splitting scheme has been used for the time integration. Then detail comparisons including stability, time step, speed, etc have been conducted. Some conclusions on the future work will be given.

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MS68

PKa Computing with Treecode Accelerated Boundary Integral (TABI) Poisson-Boltzmann Solver

pKa is an important quantity characterizing the ability of a protein active site to give up protons. pKa can be measured using NMR by tracing chemical-shifts of some special atoms, which is however expensive and time-consuming. Alternatively, pKa can be calculated by free energy changes subject to the protonation and deprotonation of an active site. The TABI Poisson-Boltzmann solver can efficiently compute free energies of solvated proteins particularly in cope with the complicated proton changes.

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MS68

Quanitfying the Conformational Fluctuation Induced Uncertainty in Biomolecular Solvation

Biomolecules exhibit conformation fluctuations near equilibrium states, inducing uncertainty in various biological properties near metastable states as well as transition between the states. We have developed a general method to quantify the uncertainty of target properties induced by conformation fluctuations. For local properties, to alleviate the high dimensionality of the conformation space, we propose a method to increase the sparsity by defining a set of collective variables within active subspace, which increases the accuracy of the surrogate model. For dynamic properties, we develop a data-driven method to evaluate the memory kernel of the energy-dissipation process based generalized Langevin Equation. The method is demonstrated on solvation properties and is generalizable to investigate uncertainty in numerous biomolecular properties.

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MS68

Accurate and Reliable Poisson-Boltzmann Solvation and Binding Energy Calculations

The ability of providing accurate and reliable Poisson-Boltzmann (PB) estimation of electrostatic solvation free energy, ΔG_{el}, and binding free energy, $\Delta\Delta G_{\mathrm{el}}$, is of tremendous significance to computational biophysics and biochemistry. In this work, we investigate the grid dependence of our PB solver (MIBPB) with SESs for estimating both ΔG_{el} and $\Delta\Delta G_{\mathrm{el}}$. Our results indicate that the use of grid spacing 0.6 Å ensures accuracy and reliability in $\Delta\Delta G_{\mathrm{el}}$ calculation.

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MS69

On Patterning and Morphology in Developmental Biology

In this talk, I will discuss the spectrum of partial differential equations that describe patterning and morphology in developmental biology. These range from reaction-diffusion equations, through the Cahn-Hilliard equation to nonlinear elasticity with differential growth. The finite element methods for the coupled solution of these partial differential equations will be described. Novel formulations of these equations hinge upon the numerical methods (in this case, finite element methods) used for their implementation.

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MS69

Simulation of Fluid-Structure Interaction Problems Arising Hemodynamics

We focus on the flow of an incompressible fluid in a compliant vessel. We propose an Arbitrary Lagrangian-Eulerian method based on Lies operator splitting. The resulting algorithm is unconditionally stable and weakly coupled: it requires the solution of one fluid subproblem and one structure subproblem, both endowed with Robin type boundary conditions, per time step. This algorithm is applied to blood flow in a healthy straight artery and in a diseased artery with implanted stent.

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MS69

A Discontinuous Galerkin Method for the Poroelastic Modeling of Intestinal Edema Formation

The loss of contractile properties of intestinal muscle tissue resulting from interstitial edema is not well understood. Experimentally validated mathematical models, based on the poroelastic Biot equations, have previously been proposed. We discretize these models using an interior penalty Discontinuous Galerkin method. The method is introduced, derived a-priori error estimates are discussed, and computational results are presented.

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MS70

Whole-Body Cardiovascular Systems Modeling of Hemorrhagic Shock

Treatment of hemorrhagic shock centers around halting bleeding and replacing lost blood volume however the differential physiological response of organs and their effect on outcome are not well understood. We are currently using a porcine experimental model and computational models of the cardiovascular system to show how cardiovascular state relates to successful resuscitation. Many of these measures of cardiovascular state can be made in the clinic giving hope of tailoring patient treatment to hemorrhagic shock.

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MS70

In-Silico Models of Neurovascular Coupling

Neurons communicate with the cerebral blood vessels to increase perfusion, termed neurovascular coupling NVC). Disordered neurovascular coupling has been observed in brain pathologies including Alzheimer's disease. Normal functioning of brain cells depends on a continuous supply of oxygen and glucose through cerebral blood flow, seen through fMRI BOLD signals. We present an in-silico model of cortical tissue allowing investigation into NVC. The model simulates ion channels, BOLD signaling, effects of vasodilators/constrictors.

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MS70

CLOCK 3111 T/C Genetic Variants Impact Circadian Regulation on Cardiac Autonomic Function

Autonomic function displays daily rhythms and plays an important role in metabolism. Humans carrying the genetic risk variant C at CLOCK (Circadian Locomotor Output Cycles Kaput) 3111T/C have greater difficulties in weight control. Here we show that the risk allele C carriers have reduced daily rhythms of cardiac autonomic activity and the reduction correlates with less efficient weight control. This work indicates the mechanistic links between sleep/circadian control, autonomic function, and weight control.

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MS71

Detection and Modeling of Structural Components Using 3D Images Derived from Cryo-Electron Microscopy

The determination of secondary structure topology is a critical step in deriving the atomic structures from the protein density maps obtained from electron cryomicroscopy technique. This step often relies on matching the secondary structure traces detected from the protein density map to the secondary structure sequence segments predicted from the amino acid sequence. Due to inaccuracies in both sources of information, a pool of possible secondary structure positions needs to be sampled. One way to approach the problem is to first derive a small number of possible topologies using existing matching algorithms, and then find the optimal placement for each possible topology. We present a dynamic programming method of $T(Nq^2h)$ to find the optimal placement for a secondary structure topology. We show that our algorithm requires significantly less computational time than the brute force method that is in the order of $T(q^Nh)$.

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MS71

Controlling 3D Structure with DNA Information

We build branched DNA species that can be joined using Watson-Crick base pairing to produce N-connected objects and lattices. We have used ligation to construct DNA topological targets, such as knots, polyhedral catenanes, Borromean rings and, using L-nucleotides, a Solomon's knot. Nanorobotics is a key area of application. We have made robust 2-state and 3-state sequence-dependent devices and bipedal walkers. We have constructed a molecular assembly line using a DNA origami layer and three 2-state devices, so that there are eight different states represented by their arrangements. We have demonstrated that all eight products can be built from this system. Wenyan Liu's empirical rule states that the best arrays in multidimensional DNA systems result when helix axes span each dimension. We have self-assembled a 2D crystalline origami array by applying this rule. We used the same rule to self-assemble a 3D crystalline array. We initially reported its crystal structure to 4 Å resolution, but rational design of intermolecular contacts has enabled us to improve the crystal resolution to better than 3 Å. We can use crystals with two molecules in the crystallographic repeat to control the color of the crystals. We can change the color of crystals by doing strand displacement of duplex DNA; we can also color the crystals using triplex formation. We are using the crystals to attempt to control the structure of other materials in 3D.

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MS71

Analyzing Biological Data via Topological Terrain

Metaphors

I will talk about the use of topological terrain metaphors for (biological) data visualization and analysis. I will in particular describe two software we developed: Denali, a generic tool for visualizing tree-like structures (such as clustering trees) using topological terrain metaphors, as well as Ayla, a specialized visual analytic tool for exploring molecular simulation data. This is joint work with J. Eldridge, W. Harvey, M. Belkin, T.-P. Bremer, C. Li, I. Park, V. Pascucci and O. Ruebel.

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MS71

Topological Method for Exploring Low-Density States in Biomolecular Folding Pathways

Characterization of transient intermediate or transition states is crucial for the description of biomolecular folding pathways, which is, however, difficult in both experiments and computer simulations. Such transient states are typically of low population in simulation samples. Even for simple systems such as RNA hairpins, recently there are mounting debates over the existence of multiple intermediate states. We develop a computational approach to explore the relatively low populated transition or intermediate states in biomolecular folding pathways, based on a topological data analysis tool, MAPPER, with simulation data from large-scale distributed computing. The method is inspired by the classical Morse theory in mathematics which characterizes the topology of high-dimensional shapes via some functional level sets. In this paper we exploit a conditional density filter which enables us to focus on the structures on pathways, followed by clustering analysis on its level sets, which helps separate low populated intermediates from high populated folded/unfolded structures. A successful application of this method is given on a motivating example, a RNA hairpin with GCAA tetraloop, where we are able to provide structural evidence from computer simulations on the multiple intermediate states and exhibit different pictures about unfolding and refolding pathways.

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MS72

Mode Conversion in the Cochlea

Mode conversion is a wave phenomenon studied in other fields such as plasma physics, geophysics, and optics. It occurs when the wave numbers of two nonorthogonal modes approach each other, and coincides with a breakdown of the WKB energy conservation equation. In the dual wave model of the cochlea, this occurs when both eigenvectors approach (-i,1). Here the identities of the modes can become confused and they may exchange energy, and also cause a reflection.

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MS72

Investigating the Spontaneous Emission of Sounds by the Mammalian Ear Using a Computational Model

The mammalian cochlea can sometimes spontaneously emit sounds, called spontaneous otoacoustic emissions (SOAEs). In this work, we investigate the generation of SOAEs using a physiologically-based computational model of the mammalian cochlea. Using our computational framework, linear stability analysis and nonlinear time-domain simulations are used to analyze the emergence of linearly unstable modes and of limit cycle oscillations. Our simulations give insights into the role of key micromechanical parameters on the generation of SOAEs.

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MS72

Intracochlear Pressure and Voltage Measurements Support Dual-Mode Cochlear Models

Recent measurements of pressure and voltage at the basilar membrane in the gerbil cochlea (Dong and Olson 2013 Biophysical J 105:1067-1078) revealed a meaningful phase relationship: At the local frequency for which nonlinearity commenced, the voltage phase underwent a transition relative to pressure. At the low frequency side of the transition, voltage was in phase with pressure and at the high frequency side, voltage led pressure by 0.3 cycle. Based on the known phase relationships between BM pressure and BM velocity, and between OHC voltage and OHC force (Frank, Hemmert and Gummer 1999 PNAS 96: 4420 - 4425), at frequencies above the transition the OHC force would be phased to pump energy into the traveling wave. Thus, the phase transition was interpreted as the activation of the cochlear amplifier. The present work has to do with the source of the significant phase transition. The voltage phase transition and accompanying amplitude variation are hypothesized to be based in OHC stimulation arising from the differencing of two modes of motion (for example, basilar membrane - tectorial membrane). Recent dual-mode models of the cochlea (Lamb and Chadwick 2014 PLOS ONE 9: e85969; Cormack, Liu, Nam and Gracewski 2015 JASA 137: 1117-1125) were used for guidance. Features of the voltage data at frequencies close to the phase transition emerged from the differencing of two traveling waves, and such a differencing is naturally available from the dual-mode models.

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MS73

Modelling with Brownian Motion on Tree-Space

Brownian motion on tree-space can be used to generate probability distributions. The simplest distributions are parametrized by a location parameter (the point the Brownian motion starts from) and a dispersion (the duration of the Brownian motion). We describe how these distributions can be fitted to collections of gene trees using Bayesian methods in order to model gene tree / species tree relationships. The methodology is applied to experimental data sets to illustrate how model fit can be assessed.

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MS73

Convex Hulls in Tree Space

Data generated in evolutionary biology and medical imaging can be tree-shaped, and thus non-Euclidean in nature, requiring new methods of analysis. One such framework is the space of metric trees constructed by Billera et al. This space is non-positively curved, with unique shortest paths between pairs of trees. Based on this property, convex hulls can be defined, and we give an algorithm for computing convex hulls in the space of trees with 5 leaves.

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MS73

Improving Quartet Based Approaches in Phylogenetics

Given the ever increasing scale of phylogenetic and phylogenomic analysis, it is important to develop scalable reconstruction algorithms. We introduce a deterministic approach for selecting representative quartet trees for use in supertree reconstruction. In addition we describe a quartet based strategy for reconstructing species trees with branch lengths.

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MS73

Developing a Statistically Powerful Measure for Phylogenetic Tree Inference Using Phylogenetic and Markov Invariants

In the late 1980's Cavendar and Felsenstein and Lake introduced the idea of phylogenetic invariants; a class of polynomials useful in the study of phylogenetic trees. Allman and Rhodes renewed interest in these polynomials taking the point of view of algebraic geometry and giving a comprehensive description of the set of polynomials which lead to their use studying numerous analytical questions like identifiability. As part of this renaissance Casanellas and Fernandez – Sanchez provided one of the first simulation studies exploring the use of the polynomials for tree inference, leaving many open questions about using the polynomials directly for tree inference. Around the same time Sumner and coauthors suggested an alternative perspective using group representation theory. We briefly present the two perspectives for the two-state general Markov model on quartet trees and then describe our study of using polynomials from each perspective to build a statistically powerful measure for tree inference, and argue for one particular measure including simulation results.

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MS74

Sleep to Save Energy or to Use Energy? Solving the Paradox

The upregulation of diverse functions, including memory consolidation and restorative processes, suggests sleep is a time for specialized energy utilization. While sleep was long considered an energy conservation strategy, the modest calculated savings led to skepticism that energy conservation is the function of sleep, particularly given sleeps inherent costs in vulnerability. Using a mathematical model, we recalculate the energy savings due to sleep and argue that energy conservation is actually the ultimate function of sleep.

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MS74

Intra- and Intercellular Roles of Hyperexcitation in Circadian Clock Neurons

Neurons in the suprachiasmatic nucleus (SCN) exhibit circadian oscillations in gene expression and membrane excitability. Previous modeling studies have shown that non-spiking hyperexcited electrical states of these neurons can support rhythmicity of the intracellular molecular circadian clock and enhance neurotransmitter signaling to other SCN neurons. In this talk I will discuss how calcium dynamics and cell morphology influence these processes.

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MS74

Mathematical Modeling of Sleep/Wake Architec-

ture in Adolescence

Sleep in adolescents is characterized by longer sleep durations and delayed timing of sleep compared to adults. To investigate mechanisms for altered sleep/wake architecture in adolescence, we adapted a physiologically-based mathematical model of the adult sleep/wake regulatory network to describe adolescent sleep. Simulated sleep reflected key features of adolescent sleep/wake behavior including the amount, timing, and architecture of sleep. Model analysis provides novel insights into the relationships between sleep physiology and dynamics.

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MS74

Explaining the Fragmentary Nature of Human Sleep Using a Sleep/Wake Model That Includes Orexin Dynamics

Healthy human sleep is punctuated by many brief awakenings, which increase in frequency towards the end of the night. Durations of sleep and wake episodes follow characteristic monotonically-decreasing probability density functions. We show here that similar distributions are generated by including noise in a recently-developed mathematical model of sleep-regulatory neural circuits in the human brain. Moreover, the statistical distributions can be understood in terms of the sleep-stabilizing orexin system and its effects on bistability.

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MS75

Role of Periglomerular Circuits in Shaping Olfactory Bulb Responses: A Modeling Study

We investigate the role of various components of the olfactory bulb circuitry in shaping the sniff-driven responses. We use network models with components constrained by adata from different cell types, and use experimentally-recorded sensory neuron responses as inputs to the model. This approach allowed us to identify circuit features underlying the temporal transformation of sensory inputs into inhalation-linked patterns of OB output. We found that realistic input-output transformations can be achieved independently by multiple circuits.

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MS75

Idealized Models of Insect Olfaction

When a locust detects an odor, the neuronal network in its antennal lobe begins oscillating. These oscillations then subside, and are replaced by slow modulations of the individual neuronal firing rates. Modeling the effects of a white-smell-type odor using an integrate-and-fire network and a firing-rate model, both with fast excitatory and inhibitory and slow inhibitory currents, we propose a possible mechanism for generating this dynamical sequence to be a slow passage through a saddle-node-on-a-circle bifurcation.

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MS75

Coding of Odors by Temporal Binding Within the Locust Antennal Lobe

The locust olfactory system interfaces with the external world through antennal receptor neurons (ORNs), which represent odors in a distributed, combinatorial manner. ORN axons bundle together to form the antennal nerve, which relays sensory information centrally to the antennal lobe (AL). Within the AL, an odor generates a dynamically evolving ensemble of active cells, leading to a stimulus-specific temporal progression of neuronal spiking. This experimental observation has led to the hypothesis that an odor is encoded within the AL by a dynamically evolving trajectory of projection neuron (PN) activity that can be decoded piecewise to ascertain odor identity. In order to study information coding within the locust AL, we developed a scaled-down model of the locust AL using HodgkinHuxley-type neurons and biologically realistic connectivity parameters and current components. Using our model, we examined correlations in the precise timing of spikes across multiple neurons, and our results suggest an alternative to the dynamic trajectory hypothesis. We propose that the dynamical interplay of fast and slow inhibition within the locust AL induces temporally stable correlations in the spiking activity of an odor-dependent neural subset, giving rise to a temporal binding code that allows rapid stimulus detection by downstream elements.

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MS75

Intrinsic and Network Mechanisms Constrain Neural Synchrony in the Moth Antennal Lobe

Projection-neurons (PNs) within the antennal lobe of the hawkmoth respond vigorously to odor stimulation, with each response followed by a ∼1s period of suppression – dubbed the 'afterhyperpolarization-phase', or AHP-phase. We investigate the mechanisms underlying this AHP-phase, and reveal some potential roles this dynamical feature might play.

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MS76

Vector-Host Models of Coinfection: Implications of Density Dependence in Vectors

Interactions among pathogen species within a host, resulting in cross protective immunity, synergistic mortality, or alterations of host infectivity or transmission can alter the dynamics of both host and pathogen populations. Whereas most coinfection models assume a constant vector population, many vectors experience density-dependent population regulation. Here we develop and parametrize a model based on a well-studied multi-pathogen, multi-vector system, barley and cereal yellow dwarf viruses (B/CYDV). Our model describes a single host, two pathogen strains, and n vector species with a single parameter describing pathogen relatedness. We examine basic (R0) and type (T) reproductive numbers, linear stability, parameter sensitivity, and the relative importance of pathogen similarity and vector population regulation on pathogen prevalence and coinfection. We demonstrate numerically that R0 describes the disease-free equilibrium stability, whereas type reproduction numbers better describe coinfection dynamics. A sensitivity analysis for two different vector growth functions indicates that infection equilibria of both formulations are sensitive to disease transmission rates, but may or may not be sensitive to vector birth and death rates and to cross protection. Thus, empirical determination of the degree and form of vector density dependence is critical for effective predictions about coinfection in natural host populations.

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MS76

Mathematical Modeling of Plants under Multiple Stressors

Plants, especially endangered species are usually affected by multiple stressors, including insects, environmental factors such as drought, and other species. Here we present a model based on a system of ordinary differential equations, and determine its equilibrium points and analyze their stability. Examples where the multiple stressors are synergistic or are anrptagonistic are presented.

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MS76

Maximizing Tree Harvesting Benefit from Forests Under Insect Infestation Stressor

Mathematical modeling has been recognized as an important tool to advance the understanding of the synergetic effect of coupled stressors (disturbances) on the forest population dynamics. Nonetheless, the state of art in the field points to a need of continuing the modeling efforts not only on addressing the link among multiple stressors but also on incorporating stressors processes. We will present an age-structured forest-beetle mechanistic model with tree harvesting. We will discuss the results of applying optimal control theory to study three different benefit functions involving healthy and dead trees in three scenarios: no beetles, beetles in endemic and epidemic states.

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MS76

Collective Intelligence-Based Early Warning in a Multi-Stressor Rice Cultivation Environment

In this presentation, we present a collective intelligence-based early warning system which assists a decision making process against in rice cultivation multi-stressors (e.g. climate, insects, plant virus) in Thailand. Such a system uses tacit knowledge collected from local farmers as well as fundamental knowledge from universities, research institutes, and government agencies. Through an assessment of how farmers explain their decision making in relation to distinct rice-related stressors; and an understanding of the set of choices available to farmers. Combined with multi-stressor sensors, the system alerts and suggests preventive and corrective actions to understand the multi-stressor causes. We present some data analysis from real farm use case, in Thailand where the local farmers are currently using our system to reduce risk rice diseases over time.

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MS77

Adapting a Classical TMDD Model into a Systems Pharmacology Approach

We describe the development of a TMDD model for Alirocumab, a pcsk9 inhibitor. Two key aspects of this development that will be discussed are: (1) adapting a classical TMDD structural model for integration into a quantitative systems pharmacology model, where some of the clearance and synthesis pathways for pcsk9 are mechanistically described, and (2) incorporating variability in drug exposure data captured in the classical TMDD model, and propagating this variability through the QSP model.

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MS77

How Complex Do Mathematical Models Need to Be in Order to Be Useful?

The last few years have seen an ever increasing use of mathematical modeling in the pharmaceutical industry. The range of these models and their applications is fairly broad. The talk will aim to provide a survey for these models, the questions they answer and if they are fit for purpose. A special attention will be paid to the use of multi-scale models of physiology and pathophysiology with special emphasis on cancer, cardio-vascular disease and osteoporosis.

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MS77

Mathematics in Cancer Therapy Development

I will present one or two applications of mathematics in drug development. The first example addresses the questions of which drugs, which doses, and what timing should be used when combining therapies. I will show how control theory is applied to an ordinary differential equation model of leukemia to optimize the potential combination regimens. A second example I may have the chance to present applies data mining techniques to predict cancer patient responses to immuno-therapy using short-term data.

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MS77

Assessing the Identifiability of Models for Monoclonal Antibody Target Mediated Drug Disposition (tmdd) Using a New Metric of Drug Potency.

We show how the parameters governing the pharmacokinetics and binding of monoclonal antibodies can be combined to provide 1) a new measure of target inhibition for multiple-dosing scenarios and 2) a lumped parameter that can be identified even when other parameters, like the baseline target concentration or the drug-target complex elimination rate, are unidentifiable.

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MS78

Spatial Pattern Formation in Microtubule Post-Translational Modifications and the Tight Localization of Motor-Driven Cargo

Microtubule (MT) "age", interpreted as nucleotide state, lattice defects, or post-translational modification (PTM) such as acetylation and detyrosination, in all three cases have been recently shown to have functionally-important effects on the dynamics of MT arrays, and can present spatial and temporal heterogeneity. While mathematical models for MT array densities are well-established, we present equations describing MT age, defined here as the mean time since the MTs building blocks (tubulin) were polymerized from their soluble dimer state. These equations use mean first-passage time calculations by adjoint-operator methods and can recapitulate the observation that the oldest (most acetylated) tubulin in axons is near the middle of axons during neuronal development in chick embryos. Furthermore, PTMs influence motor kinetics up to approximately 3-fold for off-rates and velocities. Our simulations demonstrate that this relatively weak dependence of motor kinetics is sufficient to target motor cargo to a specific location along the array. This localization is tightly peaked in a way that magnifies the relatively small signal of PTM spatial heterogeneity. Thus, MT age can produce long-range spatial patterning without feedbacks or diffusing signals.

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MS78

A Two-Protofilament Markov Chain Model of Microtubule Dynamic Instability

Microtubules offer a biological example of dynamic instability, a non-equilibrium steady-state during which catastrophe and rescue events drastically change the biopolymer's length. We present a dimer-scaled continuous-time Markov chain model of a 2-protofilament polymer, the simplest case with lateral bonds. To focus on the tip structure where most of the dynamics occur, simulated data is used to test the predictive ability of tip configurations on future growth, shortening, or stuttering events exhibited during dynamic instability.

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MS78

Mesoscopic Modeling of Polymer Transport in an Array of Entropic Barriers

In this talk, we discuss dissipative particle dynamics (DPD) simulations of the dispersion of biological polymers (e.g., DNA molecules, actin filaments, etc.) conveyed by a pressure-driven fluid flow across a periodic array of entropic barriers. We compare our simulations with nanofluidic experiments, which show the polymers to transition between various types of behaviors as the pressure is increased, and discuss physical insights afforded by the ability of the DPD method to explicitly model flows in the system. Finally, we present anomalous diffusion phenomena that emerge in both experiment and simulation, and we illustrate similarities between this system and Brownian motion in a tilted periodic potential. This is joint work with Clark Bowman, Daniel Kim, and Derek Stein.

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MS78

Microtubule Nucleation in Mitosis

During cell division, chromosomes are divided to the daughter cells by the mitotic spindle, a self-organizing structure large composed of microtubules. Microtubule nucleation is of crucial importance for cell division and spindle assembly, but remains very poorly understood due to a lack of methods capable of measuring nucleation. Here we present a methodology to bridge the large length scales accessible with microscopy and the small length scales accessible with spectroscopy, and overcome the limitation of both approaches for measuring nucleation in cells and cell extracts. We show that simultaneously acquired microscopy and spectroscopy can be used to cross-validate the models that underlie the interpretation of these techniques, thereby enabling quantitative measurements of microtubule nucleation. I will present our technique and preliminary results on the mechanism of microtubule nucleation in meiotic cell extracts.

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MS79

Near Wall Motion of Undulatory Swimmers in Non-Newtonian Fluids

Swimming and accumulation near surfaces are widely observed for microorganisms and cells, such as bacteria, C. elegans, and spermatozoa. The surrounding fluid is mostly complex and shows non-Newtonian behavior. Here, we numerically investigate the effects of non-Newtonian fluid properties, including shear thinning effects and elasticity, on the near-wall motion of microorganisms. Our results show that small amplitude undulatory swimmers are trapped near the wall, while large amplitude undulatory swimmers escape from the wall.

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MS79

Swimming Speeds of Filaments in Viscous Fluids with Resistance

We study propulsion of an infinite cylinder in a fluid with a sparse, stationary network of obstructions governed by the Brinkman equation. For fixed bending kinematics, we find that swimming speeds are enhanced due to the resistance from the obstacles. The limit for the Stokes case is recovered as the resistance goes to zero. We compare the asymptotic solutions with the numerical results obtained from the Method of Regularized Brinkmanlets.

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MS79

How Focused Flexibility Maximizes the Thrust Production of Flapping Wings

Birds, insects, and fish all exploit the fact that flexible wings or fins generally perform better. It is not clear, though, how to best distribute flexibility: Should a wing be uniformly flexible, or should certain sections be more rigid than others? I will discuss this question by using a 2D small-amplitude model combined with an efficient Cheby-

shev PDE solver. Numerical optimization shows that concentrating flexibility near the leading edge of the wing maximizes thrust production.

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MS79

Volume Effect for Particles Transported in Highly Viscous Fluids

As transporting loads is close related to objects' shapes and sizes, it is important but not trivial for researchers to determine the complexity level of models, which capture the sufficient physical phenomena. To facilitate this decision, we measure the effect of a non-zero volume spherical object transported in flows generated by nodal cilia. In our study, objects are studied in three different approaches: a passive fluid tracer, a sphere with Faxén's correction, and a detailed non-zero volume vesicle. We analyze the discrepancies in velocity field, Lagrangian trajectory and force with these three different approaches and provide qualitative information for future studies.

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MS80

Quotients of Euclidean Groups by Space Groups with Applications to Protein Crystallography

The configuration space of a rigid body is the special Euclidean group, which is a six-dimensional Lie group. This group contains 65 classes of discrete co-compact subgroups, the so-called Sohncke crystallographic space groups. The quotient of the special Euclidean group by a Sohncke group is the configuration space of a protein crystal. The properties of these spaces are explored here.

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MS80

An Energy-Law Preserving Scheme for PNP Equations

We present a numerical scheme to solve the Poisson-Nernst-Planck(PNP) equations that preserves exactly (up to roundoff error) a discretized form of the energy dynamics of the system. The equations and the energy laws are all of second-order accurate. Comparisons will be made between this energy dynamics preserving scheme and a more intuitive finite difference scheme.

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MS80

Data Driven Approaches to Molecular Biophysics

Data science has transformed our understanding of biology, but knowledge-based predictive modeling in structural biology and biophysics has lagged behind more data-rich fields such as genetics. We will present several examples of machine learning predictive models related to protein-protein binding and mutagenesis effects, allosteric communication and nucleic acid binding sites. Recasting fundamental questions about protein energetics in terms of supervised learning leads to reliable predictive models for important biophysical questions.

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MS80

Geometric and Topological Analysis of Molecular Rigidity Functions

We introduce the geometric and topological analysis for the quantitative description of molecular structures and functions. The non-smooth geometric singularities such as cusps, tips, and self-intersecting facets from molecular surface may lead to computational instabilities in the analysis and violation of the physical principle of surface free energy minimization. In our project, several techniques for molecular surface generation, curvature characterizations and electrostatic potential prediction are considered. Persistent homology analysis for curvature information, including maximum, minimun, Gaussian and mean curvatures are employed in bimolecular systems. Finally, a special binding index based on our curvature and eletrostatic information is proposed.

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MS81

Numerical Investigation of Evolution of the Biofilm Streamers

Filamentous bacterial structures, called streamers, start to form when there is a sustained hydrodynamic flow over a biofilm. In order to investigate this phenomenon, we employ a multiphase biofilm model which treats the bacteria, EPS, and background solvent as distinct phases of a complex fluid. Numerical simulations conducted reveals the impact of the viscoelasticity of the polymeric substances on the characteristics of the streamers and the complex interplay of shear flow and the bacterial filaments.

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MS81

An Immersed Boundary Method Biofilm Model with Heterogeneous Rheology

Colonies of bacteria, called biofilms, are ubiquitous in nature and, frequently grow in industrial and medical settings. Common features of biofilms include spatially heterogeneous viscosity, and a complicated viscoelastic response to material stresses and strains. In this talk, I will discuss a biofilm model based on the Immersed Boundary Method that includes variable viscosity and viscoelastic spring elements. Recent work done in validating the model with experimental data will also be presented.

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MS82

Computational Modeling of a New Paradigm for Local Blood Flow Regulation

Precise regulation of blood flow in the microcirculation is required to match oxygen supply with demand. The classical model of blood flow regulation is based on metabolic control, but mixed results from experimentation and quantitative modeling have not pointed to consensus on which specific metabolites may be responsible. A new theory proposed by Golub and Pittman in 2013 introduces an alternate paradigm, in which arteriolar vasodilation and active hyperemia are the normal state regulated by a bang-bang control that uses the signaling radicals nitric oxide (NO) and superoxide (O2-). We present a computational modeling approach to support the novel (NO/O2-)-based theory of local blood flow regulation.

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MS82

Advances in 1D Cardiovascular Fluid Dynamics Modeling

To properly understand cardiovascular dynamics associated with these changes, all aspects of the system must be considered including the fluid dynamics, the impact of the arterial wall, and the upstream and downstream vasculature. Mathematical models of the aforementioned quantities allows for prediction of pressure and flow waveforms. The biomechanical properties of the vessels change along the axial direction as well as with aging or hypertension. As vessels decrease in size, they become stiffer, an effect that is amplified by the aging process. The stiffening of vessels affects not only the wave propagation but also the shape profile of pressure waves as they travel along the vessels. Mathematical modeling can provide an essential tool for investigating how changes in wall properties and boundary conditions impact wave propagation. These models can eventually be rendered patient-specific demonstrating the changing effects on an individual. This study uses a one-dimensional fluid dynamics model coupled with a viscoelastic wall model that can predict volumetric blood flow, pressure, and vessel area waveforms in arterial networks. The viscoelastic model incorporates an elastic response as well as a creep function in describing the deformation of the arterial wall. This study used the one-dimensional model to simulate flow, pressure, and area waveforms in a large network geometry representing the ovine aorta and several of its major vessels.

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MS82

Characterizing the Pulmonary Vasculature During the Progression of PAH

Pulmonary Arterial Hypertension (PAH) is a rapidly progressive vasculopathy that commonly results in intractable right-heart failure and premature death. Transplantation of the lung remains the only cure, suggesting our limited understanding of the pathophysiology. In a controlled animal model of PAH, in vivo hemodynamic and ex vivo mechanical measurements are taken to study the dynamic vascular remodeling process. Pulmonary arterial measurements of pressure, diameter, axial length and tension obtained during ex vivo experimental setting are used to determine the tissue-level mechanical properties. These findings are incorporated into viscoelastic models to describe the dynamic changes according to arterial segments and disease stages. Our goal is to then use the in vivo hemodynamic measurements to initiate a one-dimensional fluid model and simulate the pulmonary system in health and during the progression of PAH.

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MS82

On Deriving a New Clinical Protocol for Noninvasive Assessment of the Aortic Blood Pressure Waveform Using 1D Modeling

Clinical research in creating new diagnostic tools is expensive, time-consuming and results are not warranted. We used 1D modelling to design a new clinical protocol for assessing non-invasively the central aortic blood pressure waveform from the aortic flow velocity wave. This approach produced the first demonstration of central pressure assessment based on physical phenomenon occurring in the ascending aorta. Our new protocol is currently being validated in a clinical setting.

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MS83

Medium Time Behavior of Stochastically Modeled Reaction Networks with Absolute Concentration Robustness

If the abundances of the constituent molecules of a biochemical reaction system are sufficiently high then their concentrations are typically modelled by a coupled set of ordinary differential equations (ODEs). If, however, the abundances are low then the standard deterministic models do not provide a good representation of the behavior of the system and stochastic models are used. In this talk, I will first introduce both the stochastic and deterministic models. I will then focus on models satisfying an “absolute concentration robustness’ (ACR) property. In particular, I will show how ACR models, which are stable when modelled deterministically, necessarily undergo an extinction event in the stochastic setting. I will then characterize the behavior of these stochastic models prior to extinction. This work is joint with Daniele Cappelletti and Thomas Kurtz.

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MS83

A Proof of the Global Attractor Conjecture and the Permanence Conjecture

In a groundbreaking 1972 paper Fritz Horn and Roy Jackson showed that a complex balanced mass-action system must have a unique locally stable equilibrium within any compatibility class. In 1974 Horn conjectured that this equilibrium is a global attractor, i.e., all solutions in the same compatibility class must converge to this equilibrium. Later, this claim was called the Global Attractor Conjecture, and it was shown that it has remarkable implications for the dynamics of large classes of polynomial and power-law dynamical systems, even if they are not derived from mass-action kinetics. Several special cases of this conjecture have been proved during the last decade. We describe a proof of the conjecture in full generality. In particular, it will follow that all detailed balanced mass action systems and all deficiency zero weakly reversible networks have the global attractor property. We also mention some mathematical implications for robust stability of general polynomial dynamical systems, as well as some implications for biochemical mechanisms that implement noise filtering and cellular homeostasis.

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MS83

Signs of Sensitivities in Post-Translational Modification Systems

Sensitivity analysis in chemical reaction networks comprises studying the effect that a slight perturbation exerts on the concentration of the species of the network at steady state. For instance, such a perturbation could be the addition of a small amount of one of the chemicals of the network. We want to predict the change in the concentrations of the other chemicals, after the system's return to a steady state. This information is often used for model discrimination. Since most kinetic parameters are very poorly characterized, it is often not realistic to predict the exact effects. Therefore, the goal is to predict the sign of sensitivities, i.e., which concentrations increase and which concentrations decrease as a result of the perturbation. In this talk I will show some results on the prediction of these signs, mainly focusing on post-translational modification systems. This talk is based on joint work with Elisenda Feliu.

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MS83

Multistationarity in Chemical Networks with Generalized Mass-Action Kinetics

Multiple steady states are ruled out if the right-hand-side of the dynamical system (arising from a chemical network) is injective (on stoichiometric classes). For networks with power-law kinetics, we have recently characterized injectivity in terms of sign conditions. We further extend this approach to monotone kinetics.

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MS84

Personalized Simulation of Cortical Spreading Depression

Cortical spreading depression (CSD) - a depolarisation wave originating in the visual region and propagating across the cortex to the periphery - underlays aura, a neurological phenomenon preceding migraine and causing perceptual disturbance. Numerical simulation on individual geometries obtained from MRI measurements can help planning suitable countering strategies. We present a model for the propagation of action potentials, where Diffusion Tensor Imaging (DTI) data for local conductivity information are included to improve the simulation accuracy

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MS84

Quantification of Uncertainty of Cerebral Metabolic Steady State

Identifying feasible steady state solutions of a brain energy metabolism model is an inverse problem that allows infinitely many solutions. In this talk we discuss the uncertainty in the solution, using techniques of linear algebra to identify the degrees of freedom of the flux balance analysis for a lumped model and Markov chain Monte Carlo (MCMC) methods in its extension to a spatially distributed case.

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MS84

State of the Art Combined EEG/MEG Source Analysis for Successful Presurgical Epilepsy Diagnosis

Source analysis from combined EEG-MEG data uses the complementarity of both modalities and might allow a stabilization of the reconstruction results. Taking into account the different sensitivity profiles of both modalities, requires realistic head models. This talk presents new forward and inverse techniques for combined EMEG, validated in multilayer sphere models and evaluated in realistic head models. In presurgical epilepsy diagnosis, EMEG will be shown to achieve accurate source reconstructions at early instants in time.

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MS85

Mathematical Models for Transcription and the Data Driving Them

Transcription is an important step in the process of gene expression, and a variety of mathematical models are used to describe the process. As nanotechnology extends our ability to observe structures at this nanoscale, our understanding of such systems increases, as does the model complexity. We discuss various mathematical models of transcription and the inspirations that experimental data provides, and we illustrate how the mathematical interpretation of experimental data impacts model reliability.

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MS85

Genome Organization in 3D: Formation of Chromosomal Domains in Interphase

While genomes are often considered as one-dimensional sequences, interphase chromosomes are organized in three-dimensions. Recently, chromosomal contact mapping experiments revealed Topologically Associating Domains (TADs) are fundamental building blocks in interphase. We propose that loop extrusion, where loop-extruding factors form progressively larger chromatin loops but stall at TAD boundaries, underlies TAD formation. Using polymer simulations, we find loop extrusion can produce TADs agreeing with chromosomal contact maps and reconcile observations regarding proteins related to chromosome architecture.

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MS85

They Transcribe with a Little Help from Their Friends: A Mechanistic Model for Cooperative Behavior of RNA Polymerases

In fast-transcribing prokaryotic genes many RNA polymerases (RNAPs) transcribe the DNA simultaneously. Some studies indicate that elongation seems to be faster with multiple RNAPs than elongation by a single RNAP. We have incorporated a torque mechanism into a stochastic model to explain this interaction phenomenon, and simulated transcription both with and without torque. Our results indicate the torsional interaction of RNAPs is an important mechanism in maintaining fast transcription times and efficient elongation.

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MS85

Simultaneous Regulation of Chromosome Replication and Cell Division in Bacteria

Bacteria maintain a narrow distribution of cell sizes by regulating the timing of cell divisions, but bacteria can divide faster than their chromosomes replicate. In these cases, bacteria maintain multiple ongoing replication forks by regulating the timing of initiations of chromosome replications. Here, we show that a simple model regulates simultaneously both processes. We show that the model reproduces measured correlations, distributions, and scalings in cell sizes. We also show that the model robustly maintains the correct number of replication forks in face of stochasticity in the cell cycle.

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MS86

Conformal Brain Mapping

Brain mapping uses quantitative methods to characterize shape since its highly folded nature leads to difficulty in comparing subjects. Using confomal mappings, a two-dimensional, or ‘flat,’ map of the brain can be created from medical images. We create mappings via the circle packing method to utilize certain shape aspects describing the surface structure, such as conformal invariants like extremal length. These properties can then be used to investigate anomalies in cross-subject studies.

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MS86

Oscillatory Coupling Between Prefrontal Cortex (PFC) and Hippocampus in Rodent Models of Schizophrenia

Gamma activity, aberrant in schizophrenia, is strongly modulated by low frequency oscillations, primarily responsible for dynamic coupling between distant structures. We found that these slow oscillations are generated at different frequencies in the PFC and hippocampus and oscillatory coupling may be established at either of these frequencies. We propose that the key to bidirectional coupling between PFC and hippocampus is that the interaction is frequency-tagged, i.e. the influences in different directions use different frequencies.

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MS86

Cognitive Hierarchy Across the Human Cortical

Network

Abstract not available.

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MS86

Connecting Epilepsy and Alzheimer's Disease: A Computational Modeling Framework

There are indications for strong connections between the mechanisms of Alzheimer's Disease and epilepsy. It is suggested that β-amyloid (Aβ) alters synaptic plasticity by enhanced LTD and impaired LTP. Computational models of normal bidirectional synaptic plasticity are supplemented with Aβ-induced effects to understand mechanism underlying Aβ-induced LTP and LTD. Results of both phenomenological and more detailed kinetic models help to understand the pathological mechanisms, and their role to connect epileptic seizures and impaired cognitive function.

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MS87

Phase Models and Clustering in Networks of Oscillators with Delayed Coupling

We consider a general model for a network of coupled oscillators with time delayed connections. We reduce the system of delay differential equations to a phase model where the time delay enters as a phase shift. By analyzing the phase model, we study the existence and stability of cluster solutions. These are solutions where the oscillators divide into groups; oscillators within a group are synchronized, while oscillators in different groups are phase-locked with a fixed phase difference. We show that the time delay can lead to the multistability between different cluster states. Analytical results are compared with numerical studies of the full system of delay differential equations.

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MS87

PRC Analysis of Gamma Synchrony and Clustering in Inhibitory Networks of Resonant Interneurons

Simulated sparsely coupled inhibitory networks of resonator neurons, with class 2 excitability and post-inhibitory rebound, were found to synchronize robustly with high participation rate despite heterogeneity, unlike networks of integrators. The phase response curve (PRC) of a single self-connected neuron and phase plane analyses explained why neurons either fired synchronously or skipped a cycle. The PRC with strong coupling was not type 2, but instead was linear, indicating a constant rebound that is strongly synchronizing. We also show that in cases of bistability between global synchrony and a two cluster solution, phase resetting theory under pulsatile coupling assumptions can predict the basins of attraction that determine which mode is dominant. Finally we show that in the presence of the jitter due to sparse connectivity, attractors must have a minimum width in the parameter space of conduction delays in order to be robust enough to be observed.

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MS87

Phase Models of Wave Propagation in Stochastic Neural Fields

We discuss low-dimensional approximations of nonlinear waves in stochastic neural fields with multiple layers. These phase reductions describe the position of waves in each layer of the network. Importantly, these approximations preserve information about the synaptic connectivity of the network, including the spatial heterogeneity and strength of connectivity between layers. We apply this framework to several different settings, including a path integration network with sensory feedback that corrects for errors. Our asymptotic approximations are in excellent agreement with the dynamics of the high-dimensional system.

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MS87

Weakly Coupled Oscillators in a Slowly Varying

World

We extend the theory of weakly coupled oscillators to incorporate slowly varying inputs and parameters. We employ a combination of regular perturbation and an adiabatic approximation to derive equations for the phase-difference between a pair of oscillators. We apply this to the simple Hopf oscillator and then to a biophysical model. The latter represents the behavior of a neuron that is subject to slow modulation of a muscarinic current such as would occur during transient attention through cholinergic activation. Our method extends and simplifies the recent work of Kurebayashi (2013) to include coupling. We apply the method to an all-to-all network and show that there is a waxing and waning of synchrony of modulated neurons.

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MS88

Preemptive Intervention Strategies on Community Networks

The risk of disease outbreaks within a network is important when considering where intervention strategies should be focused. The problem is intensified when considering uncertainty among regions within a network. We investigate questions of disease intervention, given uncertainty about the regions and where an outbreak occurs. We first investigate scenarios where intervention is fast, not dependent on time. We seek answers to the the problem of minimizing the costs while also lowering the expected network reproduction number below some desired threshold. We compare results to outbreak scenarios with intervention. This problem is relevant due to the current debate on vaccination campaigns and vaccine stockpiles, with questions on how many doses to be requested and where vaccines should be deployed.

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MS88

A Spatial Agent-Based Model for Feral Cats and Analysis of Population and Nuisance Control

We built an agent-based model for the survival, reproduction, and movement of feral cats and the use of trap-neuter-return (TNR) and trap-vasectomy- hysterectomy-return (TVHR) to modify cats' reproductive abilities. Spatially targeted TNR and TVHR policies are evaluated using two management goals: (1) reduce total population size and (2) reduce public nuisance. Results indicate that both TNR and TVHR have the potential to significantly reduce population size but TNR substantially outperforms TVHR in reducing nuisance behaviors.

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MS88

Brain Control - It's Not Just for Mad Scientists

It has been been hypothesized that some symptoms of Parkinson's disease are due to pathologically synchronized neural activity in the motor control region of the brain. We have developed a procedure for determining an optimal electrical deep brain stimulus which desynchronizes the activity of a group of neurons by maximizing the Lyapunov exponent associated with their phase dynamics, work that could lead to an improved control methodology for treating Parkinson's disease.

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MS88

Changing Detectors As Triggers for Immune Responses

We propose a phenomenological model in which incoherent feedforward loops play a role in immune/tumor interactions, acting as "change detectors" and complementing mechanisms of self/non-self discrimination. Acute changes are detected, but there is tolerance to constant, or even slowly varying loads. The model leads to surprising predictions regarding ranges of intrinsic tumor or pathogen growth that result in elimination versus proliferation. The IFFL motif leads to predictions of logarithmic sensing (Weber) and invariance (fold-change detection).

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MS89

Mathematics of Calorimeter

Respiration calorimetry estimates metabolic rate of organisms from the exchange of oxygen (O2) and carbon dioxide (CO2). It is modeled as a mass balance of simple set first order differential equations. These equations have been accepted since the 18th century. We will explore why applying these equations remains highly controversial because real measurements cant be proven to fit the model and many secondary effects within organisms are poorly understood.

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MS89

Evaluating the Impact of Seasonality and 'Critical Periods' in Longitudinal Studies of Growth Using Mixed Effects Models

Recent developments in modern multivariate methods provide applied researchers with the means to address many important research questions that arise in studies with repeated measures data collected on individuals over time. One such area of applied research is focused on studying change associated with periodically occurring events and critical periods in human development.

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MS89

Energy-Balance Models

Abstract not available.

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MS89

Calculating Metabolic Rate Using Kleiber's Law

Efforts have been made to derive the 3/4 power-law for many species. In this talk, we will use the relationship between the metabolic rates of species and Kleiber's law to highlight some of these efforts.

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MS90

Physiological Determinants of Response of Gout Patients to Lesinurad, a New Gout Drug, Uncovered by Modeling the Physiology of Uric Acid

We developed a compartmental model of uric acid handling by the body and calibrated it to observed data in gout patients. We simulated the effect of lesinurad on uric acid lowering in blood and concomitant increase of uric acid excretion in urine, a risk factor of kidney stone formation. Model explanation of positive benefit-risk of lesinurad in renal impaired patients in terms of uric acid physiology was used in regulatory approval of lesinurad.

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MS90

Pharmacometric Modeling and Simulation in Psychiatry

Pharmacometric approaches can be utilized to help understand not only the pharmacokinetics, but the pharmacodynamics and overall outcomes related to psychiatric illness. This presentation will highlight the application of population pharmacometric approaches to capturing individual exposures and responses to antipsychotics and antidepressants. This includes identifying drug interactions that affect the pharmacokinetics of antipsychotics such as olanzapine as well as exploring individual exposures as explanatory factors affecting the trajectory of responses in patients.

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MS90

Determinants of the Efficacy of HIV Latency Reversing Agents and Implications for Drug and Treatment Design

HIV eradication studies have focused on developing latency reversing agents (LRAs) to activate ('shock') HIV expression in latently infected cells so that these cells are purged through virus- or immune-mediated killing ('kill'). However, even in the presence of LRAs, HIV transcription may not be permanently turned on, and it is not clear which steps in the latency reversing process determine the rate of latent reservoir reduction. How drug properties affect efficacy in structured treatment regimens is not clear, and this has to be taken into consideration when evaluating candidate LRAs. We constructed a mathematical model that describes the dynamics of latently infected cells under both continuous and structured/pulsed LRA treatment. Using the model, we find that in addition to 'shock' and 'kill' rates, a previously understudied parameter, the rate at which HIV expression is deactivated both during and after LRA treatment, plays an important role in determining the efficacy of LRAs. This parameter determines the duration of HIV activation and the fate of activated cells. We further identified conditions/properties that allow LRAs to work better in structured treatment regimens than in a continuous treatment regimen. With the same amount of total dosing, pulsing treatment regimens can be more effective than a continuous treatment regimen when the 'shock' rate is high and the HIV deactivation rate after treatment stops is low.

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MS90

Understanding and Treating Periodic Hematological Disease Using Mathematical Models

Periodic hematological diseases, though rare, offer rare insight into possible mechanisms that could give rise to them. These diseases have periods ranging from weeks (cyclical neutropenia, period 13 to 65 days) to months (cyclical thrombocytopenia, period ranging from 14 to 45 days; periodic leukemia, period 37 to 83 days). This talk will survey work that has been done using mathematical models to first analyze the clinical data collected from patients, secondly to look for possible biological origins for the oscillation, and lastly to suggest new treatments for the disorders. These mathematical models typically are formulated as differential delay equations in which the delays may be state dependent and pose real challenges for their analysis and simulation. A brief survey of some of the work to be discussed can be found in Bull. Math. Biol. (2015), **77**, 739-757.

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MS91

Mathematical Modeling of Active Transport and Its Role in Cell Polarization

We review recent PDE models of active motor transport-based symmetry breaking mechanisms for cell polarization. In each case, there is some form of positive feedback mechanism involving the interaction between microtubule or actin filaments and one or more membrane-bound signaling molecules. We consider three model systems: actin polarization in spherically-shaped budding yeast, microtubule polarization in the growth cone of axons, and near-end-take-off in rod-shaped fission yeast.

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MS91

Modeling of mRNA Localization in Xenopus Oocytes

mRNA localization is essential for Xenopus egg and embryo development. This accumulation of RNA at the cell periphery is not well understood, but is thought to depend on diffusion, bidirectional movement and anchoring mechanisms. We test these proposed mechanisms using partial differential equations models and analysis, informed by parameter estimation. Our results for diffusion coefficients and transport speeds suggest different dynamics in various regions of healthy and mutant cell cytoplasm.

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MS91

Intracellular Transport: The Paradox of Codependence among Antagonistic Motors

Transport in neurons is intrinsically bidirectional, with each movement modality carried out by molecular motors in either the kinesin (anterograde) or the dynein (retrograde) families. Because all motors are present at a given time there must be competition and/or cooperation among motors that simultaneously bind a single vesicle to nearby microtubules. The prevailing tug-of-war model captures this dynamic, but fails to account for a recently recognized phenomenon: that in many situations, disabling one family of motors somehow inhibits the performance of motors that are working in the opposite direction. In this talk we will survey a few proposed mechanisms that may account for this behavior and will look at recent work that focuses on a potential role played by the helper protein dynactin.

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MS91

Mathematical Modeling of Cell Division Mechanics for C. Elegans Embryo

Cells undergo significant changes during division that require precise tuning of several mechanical events. In C. elegans embryo, the positioning of the fused nucleus in the first division cycle is remarkably well controlled and its final orientation and positioning are vital to the correct positioning of the division plane and subsequent segregation of chromosomes. In this talk we discuss a mathematical model that studies the process nuclear positioning by examining the interactions between a moving nucleus and dynamic bundles of microtubules that stochastically attach to the embryo boundary. We show that despite the complex geometry and high number of biological components needed to complete this process simple mechanical principles are responsible for remarkably robust nucleus orientation. We show that our model is well aligned with data collected from dividing embryo. This work is a collaboration with Adriana Dawes and Valerie Coffman at the Ohio State University.

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MS92

Exploring Reynolds Number Limits in the Medusan Morphospace

With a fossil record dating over half a billion years, jellyfish represent one of the earliest examples of how multicellular organisms first organized into moving systems. Lacking an agonist-antagonist muscle pairing, jellyfish swim via a process of elastic deformation and recoil. In adult (oblate) jellyfish, the Reynolds number is such that inertial forces are dominant and propulsion is generated by the interaction of vortex rings produced during the contraction and expansion of the bell. Juvenile jellyfish inhabit Reynolds number range where inertial forces are more balanced by viscous forces, and this is reflected by their drag-based swimming stroke and bell morphology. In this work, we develop an actively deforming models of adult and juvenile jellyfish immersed in a viscous fluid and use numerical simulations to describe the interplay between active muscle contraction, passive body elasticity, and fluid forces in the medusan morphospace. The fully-coupled fluid structure interaction problem is solved using an adaptive and parallelized version of the immersed boundary method (IBAMR). This model is then used to explore how mechanical and scaling properties of the bell affect the work done by the bell as well as the cost of transport related to jellyfish locomotion.

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MS92

Autonomously Responsive Pumping by a Bacterial Flagellar Forest: A Mean-field Approach

The design and fabrication of microscale pumps using magnetically actuated bacterial flagella opens the door for many applications such as the pumping and regulation of chemicals within the body. Here, we discuss simulations for a pump consisting of a regular two-dimensional array of rigid helices. Using a mean-field approach, we find the self-consistent tilt angle of the forest as a function of several parameters, and demonstrate how this pumping flow may be autonomously halted.

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MS92

Effects of Shear-Thinning Rheology on Low Reynolds Number Locomotion

We investigate the effects of shear-thinning rheology on low Reynolds number locomotion by studying a spherical squirmer in a shear-thinning fluid using a combination of asymptotic analysis and numerical simulations. We will discuss in this talk how the non-Newtonian rheological properties affect a squirming swimmer in interesting ways, where instances of both faster and slower swimming compared with the Newtonian case can occur depending on surface actuation of the squirmer.

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MS92

Patterns of Self-Propelled Rods

We first present kinetic model equations for active, anisotropic fluids arisong from biological and materials science applications. Then numerical simulation results for different parameter (active strength, polar and nematic strengths) values will be investigated. A phase diagram for stable states of active rods will be discussed with detail phase transitions.

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MS93

RNA Profiling: Extracting Structural Signals from Noisy Distributions

Accurate RNA structural prediction remains challenging, despite its increasing biomedical importance. Sampling secondary structures from the Gibbs distribution yields a strong signal of high probability base pairs. However, identifying higher order substructures requires further analysis. Profiling is a novel method which identifies the most probable combinations of base pairs across the Boltzmann ensemble. As will be shown, our combinatorial approach is straightforward, stable, and clearly separates structural signal from thermodynamic noise.

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MS93

Simulating Constrained Random Walks for Applications to Polymer Models

The fundamental model in the statistical physics of polymers is the random walk model, where the polymer's shape is assembled from random steps. Unconstrained walks with independent steps are well-understood and easy to simulate, but many biopolymers satisfy topological and geometric constraints which have proved difficult to simulate in a mathematically rigorous and computationally tractable way. We described how to use symplectic geometry to perfectly and efficiently simulate some topologically-constrained random walks, particularly cyclic walks.

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MS93

Graph Theory and Virology: Mathematics Underpinning the Discovery of Packaging Signal Mediated Assembly in RNA Viruses

Viruses face a problem akin to Levinthals Paradox in the formation of the protein shells that encapsulate their genomes: to identify the most efficient assembly pathways among the vast number of combinatorially possible ones. In this talk, we demonstrate that the solution to this problem can be formulated in terms of Graph Theory using the concept of Hamiltonian paths, revealing an evolutionarily conserved feature in the assembly of icosahedral RNA viruses.

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MS93

Fast Operator Splitting Algorithms for Biomolecular Electrostatic Analysis

Recently, we have developed several operator splitting methods to efficiently and stably solve the nonlinear Poisson-Boltzmann (PB) equation for the electrostatics analysis of solvated biomolecules. The operator splitting framework enables an analytical integration of the nonlinear term that suppresses the instability. Both fully implicit alternating direction implicit (ADI) schemes and unconditionally stable locally one-dimensional (LOD) schemes are constructed, which provide fast PB solvers in electrostatic free energy analysis.

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MS94

Multi-Scale Modeling of a Blood Clot Interaction with Fluid and Vessel Wall

A novel three-dimensional multi-scale model will be described for simulating receptor-mediated adhesion of deformable platelets at the site of vascular injury under different shear rates of blood flow. The modeling approach couples submodels of the cell membrane, stochastic receptorligand binding submodel to describe cell adhesion kinetics and lattice Boltzmann submodel for simulating blood flow. Also, macro-scale models of blood clot deformation and deformation of blood vessel will be described.

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MS94

Modeling Blood Coagulation with Rivaroxaban Under Flow

Rivaroxaban is an oral anticoagulant drug used to prevent clots from forming. There is a black box warning stating that premature discontinuation of the drug increases the risk of clotting events. This risk, which is higher than the one prior to treatment, is not fully understood. In this talk, we investigate the effects of rivaxoraban by exploring both a static and flow-based ODE model, as well as spatial-temporal PDE model of clotting.

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MS94

The Thick and Thin of It: Anticoagulation Treatment Under Flow

We use temporal models of coagulation and fibrinolytic pathways to describe injury-initiated clot formation and regression. We implement warfarin pharmacokinetics and pharmacodynamics to assess anticoagulation therapy effectiveness under normal and reduced flow conditions. We compare the results of standard clinical assessment and the biological assessment induced by simulated injury to the vessel wall. Finally, we discuss the roles of these assessment methods in the development and success of individualized treatment strategies.

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MS94

Modeling Coagulation Cascade and Blood Clotting Through a Multifidelity Algorithm

We model blood clotting by solving the PDEs associated with advection-diffusion-reaction of multiple species. Further, Force Coupling Method is incorporated to model the individual platelets. The physiological values of reaction rates, however, result in a clotting process of the order of minutes making these “high-fidelity” simulations prohibitively long. To facilitate acceleration in time, we propose a multifidelity technique using a co-krigging information fusion approach in statistical learning, which involves a few expensive high-fidelity simulations along with several much cheaper low-fidelity runs.

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MS95

Efficient Numerical Methods for the Variational Estimation of Cardiac Conductivities by Data Assimilation

The accurate quantification of cardiac conductivities is crucial for extending computational electrocardiology from medical research to clinical practice. With this motivation, we investigate a novel variational data assimilation approach for the estimation of the cardiac conductivity parameters combining available patient-specific measures with mathematical models. By resorting to a derivative-based optimization method, we significantly improve the numerical approaches in the literature. Possible model reduction techniques and steps toward validation on rabbit models will be discussed.

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MS95

A Coupled Left-Ventricle Systemic-Arteries Model

To better understand the cardio-arterial interactions, a multiscale left ventricle-systemic artery (LV-SA) model is developed, which incorporates a three-dimensional finite-strain left ventricle (LV), and a physiologically-based one-dimensional model for the systemic arteries (SA). The coupling of the LV model and the SA model is achieved by matching the pressure and flow rate at the aortic root. The governing equations of the coupled system are solved using a combined immersed-boundary finite-element (IB/FE) method and a Lax-Wendroff scheme. One baseline case, based on physiological measurements of healthy subjects, and four exemplar cases based on different physiological and pathological scenarios are studied using the LV-SA model. The results agree well with clinical observations. The developed LV-SA model can provide quantitative descriptions that are useful for understanding cardio-arterial interactions with prospective clinical applications.

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MS95

Assimilation of Patient Data in Circulation Networks for Precision Medicine in Adults and Children

Accurate lumped parameter representations of complex physiologies are typically achieved with over-parameterization. This reduces the identifiability of these systems, limiting their ability to make reliable personalized predictions. We present our recent experience in assimilating clinical data into lamped parameter circulation models under uncertainty, showing applications to single-ventricle physiologies in children, indirect estimation of pulmonary artery pressure and coronary bypass graft hemodynamics in adults.

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MS95

Predicting Cardiovascular Dynamics for Surgical Planning in Several Congenital Heart Diseases

Blood flow simulations for surgery planning are typically based on preoperative patient data. We will present strategies to parameterize multiscale models based on the type of available data. Then we will show through different examples of congenital heart diseases, which hemodynamics changes due to surgery or intervention have been predicted. Finally, we will discuss validation, when possible, of the models.

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MS96

On the Existence of Positive Steady States for Weakly Reversible Mass Action Systems

A long standing question in Chemical Reaction Network Theory is whether the weak reversibility of the underlying network of a mass action system is sufficient to the existence of positive steady states in each of the positive stoichiometric classes. Recently, Deng, Feinberg, Jones, and Nachman proposed a proof of this conjecture. In this talk, we will discuss the main ideas of their manuscript.

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MS96

Conditions for Multistationarity and Switching in Mass Action Networks

Multistationarity and switching have been recognized as important features of dynamical systems originating in

Biology. Often these properties are established numerically. However, parameter uncertainty complicates numerical analysis. Hence techniques allowing the analytic computation of parameters where a given system exhibits either multistationarity or switching are desirable. We present conditions in form of polynomial systems that allow to determine parameter vectors where a mass action system exhibits multistationarity or switching. These polynomial systems arise from the structure of the reaction network and hence are not affected by parameter uncertainty.

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MS96

Identifying Multistationary Reaction Networks

It is an open problem to identify reaction networks that admit multiple positive steady states. Criteria such as deficiency theory and Jacobian criterion help rule out the possibility of multiple steady states. But these tests are not sufficient to establish multistationarity. For fully open networks, we can establish multistationarity by relating the steady states of a reaction network with those of its component embedded networks. We refer to the multistationary fully open networks that are minimal with respect to the embedding relation as atoms of multistationarity. We identify some families of atoms of multistationarity and show that there exist arbitrarily large (in species, reactions) such atoms.

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MS96

Necessary and Sufficient Conditions for Multistationarity in Networks of Interacting Elements

Starting from ideas of Craciun and Feinberg, we discuss some old and new necessary and sufficient criteria for injectivity and multistationarity in vector fields associated with interaction networks. The results are phrased in a common matrix-theoretic setting, and connections with graph-theoretic corollaries also discussed. This is joint work Murad Banaji (University of Portsmouth).

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MS97

Electro-Metabolic Activity of the Neuron-Astrocyte Complex: Mathematical and Numerical Coupling

Computational models are more relevant than ever to draw a comprehensive picture of the working human brain, where several dynamics coexist at different temporal scales. We propose a model that couples the electrophysiological activity of the neurons, the metabolic cycle of the neuron-astrocyte complex, and the nutrient supply from capillaries irrigating the cerebral tissue. We address mathematical and numerical aspects of integrating the different time scales at play: the millisecond (electrophysiology), and the second (metabolism).

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MS97

Identification of Vasodilatory Stimulus from Cerebral Blood Flow Data

The BOLD signal in functional MRI imaging is a consequence of the vasodilatatory signal from an activated neuron/astrocyte complex. In this presentation, we address the question of how to estimate the stimulus signal from the CBF data, and the identifiability of the vascular compartment (arterial/capillary/venous)responsible for the BOLD signal.

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MS97

Computer Aided Clinical Trials and Surgical Planning in Cerebral Aneurysms: Challenges and Perspectives

Numerical modeling of cardiovascular problems is nowadays at the stage of becoming a tool to support decisions of physicians in the clinical practice. Cerebral aneurysms have attracted the interest of many researchers in this field, with different contributions in fluid and structural mechanics, and image processing. We review some of these contributions in the perspective of clinical routine, both to extract knowledge as in Clinical Trials and to help doctors for an effective Surgical Planning.

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MS97

Computation of Brain Deformations for Image-Guided Neurosurgery: Progress and Uncertainty

We show that sufficiently accurate prediction of the brain deformations during surgery can be achieved when the load is defined by prescribing the displacements on the exposed (during surgery) brain surface formulation known as displacement-zero-traction problem of computational mechanics. For this formulation, the computed deformations within the brain are for practical purposes insensitive to uncertainty in the information about patient-specific properties of the brain tissues. We demonstrate that accurate prediction of the organ (brain) deformations can be achieved by means of patient-specific biomechanical models generated in semi-automated manner directly from medical images using the concept of medical-image-as-a-biomechanical model. This concept utilises Galerkin-type meshless discretisation of equations of solid mechanics and statistical tissue classification to assign the constitutive parameters at integration points of computational grid. While acknowledging the progress achieved in computational biomechanics for image-guided surgery, we open discussion on topics that, in our opinion, have not been given sufficient attention by the biomechanical community. These include the effects of uncertainty (due to limited resolution and quality of the available imaging techniques) when determining loading (organ surface displacements) from medical images and very limited quantitative data about boundary conditions for the brain and other body organs.

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MS98

Turing Patterns from "Differential Growth": A Minimal Model for Pattern Formation in Zebrafish Skin

The core mechanism of pattern formation on zebrafish skin seems affected by an apparent intrinsic contradiction: the patterns behave like Turing patterns, but evidence shows the absence of a reaction-diffusion mechanism. Here we show a minimal model based on the available experimental information, which is able to produce Turing patterns without diffusion or any other cellular motion. This model unveils a completely new mechanism for the zebrafish pattern formation, which we name "differential growth".

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MS98

Cellular Basis of Color Pattern Formation in Zebrafish

Animals display remarkable colour pattern diversity; colour patterns are highly variable and evolve rapidly leading to diverse coloration even within closely related species and to remarkable similarities in distant genera. The cellular and molecular mechanisms underlying pattern formation in vertebrates are not well understood. An understanding of the patterning mechanisms will be important in deciphering the genetic basis of pattern variation in evolution. The zebrafish striped coloration has become an important vertebrate model to investigate mechanisms underlying pattern formation in a nearly 2-dimensional system by using interdisciplinary approaches. The striped coloration arises from a layered arrangement of three pigment cell types - yellow xanthophores, silvery or blue iridophores and black melanophores. By long-term imaging over several weeks and lineage tracing, we analysed cellular origin and cell behaviours underlying stripe pattern formation in zebrafish. The melanophores and the iridophores originate from peripheral nerve-associated postembryonic progenitors whereas most adult xanthophores originate from local proliferation of larval xanthophores. The precise organisation of the three cell types into a striped pattern emerges from cell-cell interaction dependent coordinated cell movements, cellular reorganisations and cell shape transitions.

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MS98

Agent-Based Models of Stripe Formation on Zebrafish

Zebrafish (Danio rerio) is a small fish with distinctive black and yellow stripes that form due to the interaction of different pigment cells. Working closely with the biological data, we present an agent-based model for these stripes that accounts for the migration, differentiation, and death of three types of pigment cells. The development of both wild-type and mutated patterns will be discussed, as well as the non-local continuum limit associated with the model.

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MS99

Mathematical Descriptions of Bipolar I Patients from Longitudinal Patterns of Mood

Bipolar disorder is a chronic disease of mood instability. Longitudinal mood patterns are central to patient descriptions, but are reduced to simple attributes. Models could provide more nuance, but there is little justification on what that model should be. Combining inferences across 197 patients, we find no evidence to support assumptions that mood is one-dimensional, rhythmic, or multistable. We introduce a model that reflects the data, reproduces clinical features, and can be personalized.

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MS99

A Turing Pattern Formation Model of Cortical Folding

Individual variability in the folding pattern of the human brain begins early in development. It is not understand how or why the folds develop where they do. We present a Turing reaction-diffusion model of cortical folding. By altering various model parameters, including domain size and scaling, results from our model can be correlated with cortical folding diseases such as lissencephaly and microcephaly. This model demonstrates some of the key factors involved in cortical folding.

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MS99

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Abstract not available.

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MS99

Interactions Between Electrophysiology and Neuropharmacology

Psychiatric illnesses are often treated with drugs that change the chemistry of the brain. But how do local chemical changes affect the electrophysiology of brain and vice versa? My colleagues, Janet Best and Fred Nijhout, and I create mathematical models to study volume transmission in which neurons in a nucleus project to a distant nucleus and influence the electrophysiology there be changing the local biochemistry instead of by one-to-one neural transmission.

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MS100

Synchronization of Spiking and Subthreshold States in Electrically Coupled Networks of Neurons

Subthreshold oscillations and spiking coexist in many brain regions, including the inferior olive. Electrical coupling has been shown to synchronize both states. We explore differences in their phase locking properties using the resonate-and-fire model. We present a technique to calculate the iPRC, construct phase-reduced models, and assess the stability of synchrony. We show that the while the spike itself promotes synchrony, the post-spike reset can oppose it, representing a trade-off for neural systems.

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MS100

Clustering in Inhibitory Neural Networks with Nearest Neighbor Coupling

In this talk, I will discuss some recent development on the clustering dynamics of a network of inhibitory interneurons. Specifically, the phase model analysis is used to study the existence and stability of cluster solutions; the precise conditions for the stability of these solutions are derived for nearest neighbor coupling. The results show that changing the connection weights in the network can change the stability of cluster solutions in inhibitory networks.

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MS101

Optimal Harvesting Strategies for Timber and Non-Timber Forest Products in Tropical Ecosystems

We apply optimal control theory to investigate optimal strategies for the combinations of non-lethal (e.g., NTFP) and lethal (e.g., timber) harvest that minimize the cost of harvesting while maximizing the benefits (revenue) that accrue to harvesters and the conservation value of harvested ecosystems. Optimal harvesting strategies include starting with non-lethal NTFP harvest and postponing lethal timber harvesting to begin after a few years. We clearly demonstrate that slow growth species have lower optimal harvesting rates, objective functional values and profits than fast growth species. However, contrary to expectation, the effect of species lifespan on optimal harvesting rates was weak suggesting that life history is a better indicator of species resilience to harvest than lifespan.

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MS101

Management Strategies in a Malaria Model Combining Human and Transmission-Blocking Vaccines

A new mathematical model studying control strategies of malaria transmission is formulated and analyzed. The ex-

istence of a backward bifurcation is established analytically in the absence of vaccination, and numerically in the presence of vaccination. Optimal control strategies, using vaccination and vector control are investigated to gain qualitative understanding on how the combination of vaccination and vector control should be used to reduce disease prevalence in a malaria endemic setting.

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MS101

Optimal Control Applied to a Differential Equation Model for an Anthrax Epizootic

Anthrax is a fatal disease caused by a gram positive, spore forming bacteria called *Bacillus anthracis*. The disease is endemic to several national parks and one of the main causes of herbivore decline. Most anthrax infected animals face inevitable death and each infected carcass deposits massive number of spores into the surrounding environment. Thus, controlling new infections through vaccination and eliminating spread through proper carcass disposal are the only feasible ways to effectively control the disease when an outbreak occurs. In this talk, a system made up of parabolic partial differential equations together with ordinary differential equations will be presented and introduction of the two most commonly used controls of vaccination and carcass disposal into the system will be investigated. We determine the effect that these two control measures have on disease transmission and cost using optimal control theory. Parameter sensitivity and numerical results will also be presented.

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MS101

Using Optimal Control Theory to Analyze the Treatment of a Bacterial Infection in a Wound with Oxygen Therapy

A mathematical model describing the interactions of bacteria, inflammatory cells, and oxygen in a wound describing the treatment of a bacterial infection using oxygen therapy will be presented and analyzed. A second variation of the model will be presented in an optimal control setting with the control variable being the input of supplemental oxygen. Numerical results of the optimal control model will be presented and future directions will be discussed.

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MS102

Modeling Accelerometer Signals from Wearable Physical Activity Monitors

Obesity results from net positive energy balance (intake¿expenditure) over time. With increasing interests in quantifying energy expenditure and technical advancements in portable physical activity monitoring devices, the need to develop models to translate accelerometry data into energy expenditure is critical. We will explore the past and current approaches ranging from simple linear regressions to machine learning algorithms (artificial neural network) and discuss future needs for moving this field forward.

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MS102

Modeling to Predict Childhood Obesity Trends in School

School-based interventions provide the best obesity prevention and reduction strategy in children. Evaluating the isolated effectiveness of an intervention in light of changing height and body composition is challenging. Additionally, physiological and psychosocial responses to an intervention are dependent on baseline body mass index (BMI), sex, socioeconomic status, and age. We use mathematical models to quantify expected school specific BMI trends and determine how and if the BMI trajectory was altered due to the intervention.

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MS102

Application of Mathematical Models in Management of Obesity in Prenatal and Postnatal Care

Abstract not available.

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MS103

Granulopoiesis Physiology Determines the Pharmacokinetics of Granulocyte Colony-Stimulating Factor (G-CSF)

Pharmacokinetic (PK) models are generally constructed relying upon clinical data for their determination. Unfortunately, this approach may obfuscate or ignore physiological principles which dictate the behaviour of a drug in the body. Here I will discuss a novel PK model which we have developed for granulocyte colony-stimulating factor, an endogenous cytokine administered exogenously to treat a variety of granulocyte pathologies, which explicitly incorporates specific removal mechanisms and tracks both bound and unbound blood concentrations.

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MS103

Modelling the Pharmacodynamic Effects of Granulocyte Colony-Stimulating Factor on Granulopoiesis

The production of white blood cells is modelled from hematopoietic stem cells (HSCs) through proliferating and maturing precursors to circulating neutrophils. The main cytokine that regulates this process is Granulocyte Colony Stimulating Factor (G-CSF). We use G-CSF concentrations to regulate the differentiation rate of HSCs, the proliferation rate during mitosis, the maturation time, and the rate at which mature neutrophils are released into circulation from the bone marrow. The variable maturation time is modelled via an age-structured PDE model with variable ageing rate which results in state-dependent delays, and we also show how these arise.

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MS103

Web Accessible Population Pharmacokinetics Service - Hemophilia (WAPPS-Hemo): an innovative approach to tailored prophylaxis

The WAPPS-Hemo project aims to develop a web-accessible service to assess pharmacokinetics of clotting factors used in hemophilia treatment. Brand-specific models were generated using rich data from industry sponsors and a population pharmacokinetics approach, and individual PK estimates can be produced from only a few samples. Twenty-two clinical centres have registered to participate in the development and testing phases of the project. Overall, WAPPS-Hemo constitutes an innovative blend of approaches to tackle a rare disorder.

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PP1

Mathematical Morphological Distribution Properties Over Union and Intersection

Mathematical Morphological Concepts outlines techniques for analysing and processing geometric structures based on set theory. We present theorems on morphological distributions properties over unions and intersections with respect to Dilation and Erosion. Our results show that both dilation and erosion are distributive over unions but non-distributive with respect to intersections

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PP1

Macroscopic Dynamics of Heterogeneous Theta Neurons Connected with Chemical Synapses

The theta model is useful for the investigation of the population dynamics of coupled neurons due to the periodic boundary conditions of the corresponding Fokker-Planck equation. However, the effects of heterogeneity in the population has not been thoroughly explored. Here, we propose a heterogeneous version of modified theta model, and investigate the population dynamics by Ott-Antonsen ansatz. Then we analyze the macroscopic phase response functions of excitatory and inhibitory neuronal populations

of the proposed model.

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PP1

Multiple Chronic Conditions (MCC) Along the US-Mexico Border

Little is known about MMC and their occurrence in older adult patients, especially in the US-Mexico border. We investigated multiple chronic conditions among the US-Mexico border aged population and patterns of multimorbidity using data mining. For the purpose of this pilot study 50 model alternations have been tested on a small sample, each represented by an individual process in rapidminer data mining tool. The top algorithms that gave the best results were classification algorithms.

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PP1

An Age-Structured Model for Cyanobacteria Carboxysome Efficacy

Cyanobacteria are photosynthesizing microorganisms lauded as worthwhile possibilities for cleaning excess CO2 from earths atmosphere, creating biofuels and allowing sustainable outposts on Mars. The enzymes required for photosynthesis, and thus carbon fixation, are encapsulated into structures called carboxysomes. The age-structured model presented in this work provides insight into the influence of carboxysome senility on carbon fixation performance in cyanobacteria. Increased understanding of this link could elucidate targets for engineering cells with improved photosynthetic capability.

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PP1

Protein Dynamics in Curved Lipid Bilayer Membranes: Fluctuating Hydrodynamic Methods for Manifolds

We present theory for protein diffusion and active transport within curved lipid bilayer membranes. Our theory takes into account the hydrodynamics within the two bilayer leaflets, intermonolayer slip between the leaflets, and coupling with the surrounding bulk solvent fluid. In 1975, Saffman and Delbruck introduced a hydrodynamic theory for infinite flat sheets that is still a widely used theory for the diffusivity of membrane proteins. We show for a finite curved membrane sheet that geometric and topological effects can significantly augment the protein diffusivity and hydrodynamic coupling. We present results showing how these effects contribute to the individual and collective motions of protein inclusions in spherical vesicles. We also present general fluctuating hydrodynamic methods for manifolds that can be used for general investigations of many-body systems involving diffusion and hydrodynamic transport within thin fluid interfaces having curved geometries.

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PP1

Symmetric Proteins from Asymmetric Sequences: Lessons from the β-Propeller Fold

Repeat proteins are characterized by distinctive structural repetitions, which often arise from gene duplication events, facilitating the expansion of these protein families. Despite the high similarity in three-dimensional conformation for each repeating region, different repetitions in these protein families often have (and require) variation in primary structure. We demonstrate how computational protein design algorithms can be adapted to explore the influence and necessity of sequence variation in the radially symmetric β-propeller fold.

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PP1

An Inverse Problem for a Time Varying Diffusion

Process

We investigate a stochastic differential equation that models diffusion of a membrane-targeting protein on the surface of a cell. In this model, the diffusion coefficient governing the protein's movement is assumed to switch in time between discrete quantities, corresponding to different binding configurations of the protein under study. We propose a method to deduce both the underlying diffusion coefficients from a given sample trajectory and determine the times at which the switches occur.

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PP1

Quantifying the Potential of Immunotherapy in Combination with Androgen Ablation for the Treatment of Prostate Cancer

Androgen ablation therapy is a treatment used in early stages of prostate cancer. However, the cancer usually recurs and is resistant to this initial treatment. New treatments have been developed, such as immunotherapy, which use the patients own immune system to target the tumor. New evidence points to using a combination of these two treatments. We will investigate this using a mathematical model that includes temporal dynamics of key cells and chemokines, and drug action.

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PP1

Walking of a Single Walker and a Pair of Walkers in the Absence of Orientation Cues

Vision and hearing are used as geographical cues by humans in order to navigate to a target. We propose a mathematical model of human walk in the absence of navigational cues based on a parametric family of stochastic difference equations with individual-based parameters. Furthermore, we study how accuracy of walk under such conditions can improve if humans walk in pairs. Theoretical predictions of the models are compared with numerical simulations and experiments with humans and robots.

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PP1

Mathematical Modeling of Endotoxin-Induced Inflammatory Response in Young Men

The magnitude of an acute inflammatory response is of critical importance in evaluating patients during early postoperative mobilization. Uncontrolled inflammation can cause further tissue damage; insufficient inflammation can result in immunodeficiency. An uncontrolled inflammatory response can cause further tissue damage, while an insufficient response can result in immunodeficiency. Here, we present a mathematical model incorporating key components of the inflammatory response in humans. Our model was calibrated to experimental data obtained from experiments measuring pro-inflammatory cytokines (IL-6, IL-8, and TNFα) and the anti-inflammatory cytokine IL-10 over 8 hours in 20 healthy men, given a low dose of lipopolysaccharide (LPS), an endotoxin stimulating inflammation.

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PP1

Theoretical and Numerical Study of Cardiac Electrophysiology Problems at the Microscopic Scale

The bidomain model efficiently represents macroscopic cardiac electrophysiology but neglects inhomogeneities on the cellular scale. Furthermore, it cannot represent gap junctions accurately. We introduce a microscopic model. We prove the existence of a solution of this model. Numerical simulations in a 3D model of two cells will be shown as a first step to reach several cells.

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PP1

Mathematical Modelling Based Hypothesis for the Origins of Cyclical Neutropenia

Cyclical neutropenia is a dynamical disease resulting in oscillations in circulating neutrophil populations. Previous mathematical models predict that the disease results from decreased amplification of maturing cells, but modelled the amplification process in limited complexity and did not offer an explicit physiological defect responsible for the decrease. We study a new model which differentiates between the different mechanisms involved in amplification and produce a hypothesis for the specific physiological process leading to the oscillations.

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PP1

Polyrhythmic Pattern Generation in Networks with Three-Node CPG Kernels

Inhibitory Fitzhugh-Nagumo-type networks of 3-cell motifs may produce phase-locked states: pacemakers, traveling waves, peristaltic rhythms, and recurrent phase-varying lags. Reduction of coupled dynamics to low-order phase maps permits broader exploration of network repertoire, aiding search of biologically relevant parameters resulting in robustness of patterns observed in nature. We identify multi-stable rhythms within a single network, with rhythm switching, permitting direct and testable hypotheses underlying basic features of a number of identified networks with 3-cell kernels.

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PP1

A Mathematical Model of Blood Flow Control in the Kidney

The mammalian kidney maintains the balance of water, salt and blood pressure of the body. A published model simulates hemodynamic control in the kidney by representing the interactions between autoregulatory mechanisms, including the myogenic response, the tubuloglomerular feedback and the connecting tubule glomerular feedback. In this study we aim to extend that model to include more realistic tubular water transport, and to apply that model to investigate the origin of renal blood flow oscillations.

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PP1

Understanding the Finite State Projection and Related Methods for Solving the Chemical Master Equation

The ?nite state projection (FSP) method of Munsky and Khammash has enabled us to solve the chemical master equation (CME) of some biological models that were out of reach not long ago. Since the original FSP method, much effort has gone into transforming it into an adaptive time-stepping algorithm. Some improvements include the multiple time-interval FSP and most notably the Krylov-FSP approach. The poster will give an overview of these current methods.

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PP1

A Reduced Model of Cardiac Ion Channel Pharmacology

Cardiotoxicity of many pharmaceutical drugs often results from alterations in ion channel kinetics. While detailed ion channel models accurately capture the conformational state-specific affinities of these problematic drugs, the complexity of these models makes tissue-level simulations expensive and prohibits identification of mechanisms of cardiotoxicity. We present a reduced model of the cardiac sodium channel $\mathrm{Na}_v1.5$ that overcomes the limitations of detailed models, and we assess its feasibility for predictive pharmacology.

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PP1

Identifying Leading Gene Expression Features to Distinguish Snps Causative of Disease

The completed human reference genome has allowed for multitudes of Genome wide association Studies (GWAS), which have identified tens of thousands of single nucleotide polymorphisms (SNPs) that are correlated with the presence of complex disease. Several features of genes and genomes, including sequence conservation have been developed for prioritizing likely-causative SNPs for further interrogation, but efficiently prioritizing SNPSs remains an open problem. Identifying influential SNPs that reside in the non-coding portion of the genome is particularly challenging due to the fact that there are minimal ways to interpret the non-coding sequence. Given that the majority of disease-causing SNPs are believed to fall in the noncoding genome, this problem is of particular importance. Because it is known that non-coding sequence influences the regulation of gene expression, we hypothesize that gene expression can be an informative feature in prioritizing SNPs. With the recent advances in RNA-sequencing, we now have gene expression data available for hundreds of humans across many of cell types. In addition, the Broad Institute has recently sequenced RNA-seq data of 9 mammals across 12 tissue types, which allows us to characterize evolutionary patterns of gene expression. With this newly available data, we are able to analyze the relationship of the disease and non-disease-causing SNPs to expression features of nearby genes and discover informative SNP prioritizing features.

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PP1

Sex Differences in the Electrical Properties of Neurons in the Neural Song System of the Zebra Finch

Zebra finches have a highly sexually dimorphic neural song system. Our electrophysiology studies indicate sex differences in features of key neurons in the song system. Are these due to differences in the expression level of ion channels, or due to variation in the kinetics of the channels? We use a modeling approach and the dynamic clamp modeling/experimental technique to explore the biophysical basis of differences in the electrical properties of these neurons.

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PP1

Analysis of Neural Network Models for Sequential Activity

The neural circuitry that drives song production in oscine songbirds has been studied extensively as a model for the generation of learned behavior. Nucleus HVC, a central component of the song system, contains a temporal code for song in a circuit which indirectly controls the generation of adult song. In this study, we build on neural network models which describe this circuit, study their properties, and derive predictions based on their behavior.

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PP1

Nonlinear Microwave Imaging for Breast-Cancer Using a Variational Bayesian Algorithm

Microwave imaging is becoming a promising alternative technique to current imaging modalities since it offers a significant dielectric property contrast between normal and malignant breast tissues. Microwave imaging is considered as a nonlinear inverse scattering problem and is tackled in a variational Bayesian estimation framework based on a prior modeling key which implies that the object under test is assumed to be composed of compact regions made of a restricted number of different homogeneous materials.

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PP1

Homogenisation Theory with Coupled Cellular Reaction Diffusion Equations

Disturbed vision experienced prior to migraine is known as an "aura'. Visual auras are thought to be caused by a slow moving large amplitude wave, consisting of K^+ ions traversing the occipital lobe in the brain, is termed Cortical Spreading Depression (CSD). A coupled cell model based on the work of Goldbeter et al. (1990) was developed using homogenisation theory. Coupling simulated both Fickian and electro-diffusion. Complex patterns emerged particularly where the coupling varied spatially.

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PP1

Recovery Rates in Epidemiological and Ecological Models

Differential equation models of infectious disease have undergone many theoretical extensions that have proved invaluable for the evaluation of disease spread. For instance, while one traditionally uses a bilinear term to describe the incidence rate of infection, physically more realistic nonlinear generalizations exist. However, such theoretical extensions of recovery rates have yet to be developed. This is despite the fact that a constant recovery rate does not perfectly describe the dynamics of recovery, and that the recovery rate is arguably as important as any incidence rate in governing the dynamics of a system.
To address this void in theoretical development, we provide a first principle derivation of nonlinear recovery rates in differential equation models of infectious disease. To accomplish this, we rely on an intimate connection between integral equations, stochastic processes, and differential equations. Finally, we outline the benefits of a novel state dependent recovery rate, where infected individuals can only contribute to disease spread for a finite amount of time, in comparison traditional constant recovery rates.

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PP1

Numerical Exterior Calculus Approaches for Hydrodynamics on Curved Surfaces

We discuss how exterior calculus approaches can be used to formulate models of hydrodynamic flows on curved surfaces. We consider two-dimensional star-shaped surfaces having spherical topology embedded in R^3. We show how spherical harmonic representations can be used to develop numerical methods based on discrete approximations of the exterior calculus operators, such as the co-differential, exterior derivative, and Hodge star. We then present results demonstrating our approach on a few applications.

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PP1

A Mathematical Study of Calcium Responses in HSY Cells and Airway Smooth Muscle Cells

A salivary ductal cell line (HSY) exhibits oscillations in the cytosolic calcium concentration that are about 15 times slower than those in airway smooth muscle cells. However, both cells respond in a qualitatively similar way to photolysis of caged IP_3, showing anomalous delays in their calcium responses. We present a mathematical model of calcium dynamics and show that both oscillatory processes share dynamic similarities, despite the significant difference in their periods.

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PP1

Investigating Experimental Variations in Astrocytes with a Mathematical Model of Calcium Dynamics

Astrocytes are the most common glial cells in the brain, communicating via calcium transients, and possibly modulating neuronal signals. We explain experimental variability with a new open-cell mathematical model by studying the various fluxes through calcium channels. We show the surprising result that fluxes that do not play an active role during calcium transients still have the ability to affect the underlying phase space of the system, and thus the shape of the calcium transients.

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PP1

Using the CUR Factorization to Identify Key ECG Morphologies

The goal of this work is to identify key beat morphologies within pediatric electrocardiogram (ECG) recordings – specifically those of patients with congenital heart disease – for future use in developing predictive models. To do so, this work uses the CUR factorization with incremental QR. The sensitivity of CUR to different types of morphology variations is first tested on synthetic ECG data, and then preliminary experiments are performed on a small subset of real patient data.

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PP1

Spatiotemporal Organization of an RNA Polymerase Along a DNA Strand

The first crucial step in gene expression is the transcription of the DNA to the RNA. One can think of this step as a movement of a complex machine, an RNA polymerase, on a one-dimensional template strand. We have developed a mathematical model to explore the spatiotemporal organization of an RNA polymerase along the DNA strand. We have found the probability density profiles, the mean velocity and other statistical properties related to one RNA polymerase.

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PP1

A Re-Evaluation of the Concept of Critical Concentration as it Relates to Microtubules

Classic understanding of monomer-polymer relationships in cytoskeletal polymers derives from equilibrium systems, where the 'Critical Concentration' (Cc) of monomers needed for polymer assembly is accepted to be a single value with several equivalent definitions. Using computational modeling, we show that the varied definitions of Cc yield empirically different values for Cc, each with practical implications. This has significant implications for the design and interpretation of microtubule experiments and likely has relevance to any steady-state polymer.

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PP1

Persistant Neural Response in the Aplysia Bag Cell Neuron

Persistent neural response is a mechanism by which a brief stimuli can induce long-term firing behavior in the nervous system. Qualitative similarities in persistent neural responses are prevalent across species, including motoneurons in turtles, the escape response of lamprey, and numerous cortical regions relating to memory and attention. Persistent activity is often associated with peptide release, as is the case with mammalian maternal function in birth and lactation through the release of oxytocin. Here, we develop an ion-conductance neuron model to reproduce persistent behavior in Aplysia reproduction. In Aplysia, bag cell neurons in the abdominal ganglia respond to a brief pulse with persistent neural oscillations, known as the afterdischarge, inducing the release of peptides associated with egg-laying. After several minutes of persistent activity, the neuron transitions to a refractory period where it can function as a normal threshold neuron, but afterdischarge cannot be invoked until the refractory period ends. Mounting evidence suggests intrinsic cellular mechanisms, namely calcium, are responsible for the transition to persistent oscillations and the refractory period. Development of the Aplysia bag cell model is in collaboration with the experimental lab of Neil Magoski at Queen's University, which provides data and insightful observations to inform the development of the mathematical model.

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PP1

Chemotactic Response Models for Motile Bacteria

Phenomenological models for the chemotactic response of bacteria such as E. coli generally support the formulation of a Keller-Segel PDE model for the bulk response, with the chemotactic drift velocity linked to the local gradient of the attractant and a random motility that is invariant. These results are for the limit of a weak response by the cell and the drift velocities are lower than commonly seen in experiments. We report on models for a stronger cell response, how variations in the models affect outcomes and the link to cell processes.

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PP1

Onset, Timing, and Exposure Therapy of Stress Disorders: Mechanistic Insight from a Mathematical Model of Oscillating Neuroendocrine Dynamics

Disruptions in the neuroendocrine activity of the hypothalamic-pituitary-adrenal (HPA) axis are correlated with stress-related diseases such as post-traumatic stress disorder and major depressive disorder. In this paper, we characterize "normal" and "diseased" states of the HPA axis as basins of attraction of a multiple-time-scale dynamical system describing the inhibition of peptide hormones such as corticotropin-releasing hormone and adrenocorticotropic hormone by circulating glucocorticoids such as cortisol.

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PP1

Altered Excitatory-Inhibitory Dynamics by a Feedback Loop with Long Delays

In this study, we examined how feedback signal relayed by an additional excitatory population (E_1) may alter the critical coupling strength required to generate oscillations within an excitatory-inhibitory network (E_2I_3). We find that as the transmission delay between E_1 and E_2I_3 is varied, the critical coupling strength of E_2-I_3 loop modulates with wide amplitude, on the other hand, the I_3-I_3 loop oscillations are robust to the changes in the delay.

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PP1

Quasi-Steady State Approximation for Reversible Bimolecular Binding with Application to Alternative Mechanism of Telomere Length Maintenance

The quasi-steady state approximation (QSSA) is com-

monly applied in chemical kinetics without its rigorous justification. We show that the detailed analysis of dynamics of evolution of telomere length without the presence of telomerase requires QSSA in a large number of reactions. We provide a justification of such QSSA for individual reactions in a general case of reversible two-step bimolecular binding in two different regimes: under the symmetrized Briggs-Haldane criterion and under an alternative condition. The derived conditions may be of practical use as they provide weaker requirements for the validity of QSSA compared to the existing results.

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PP1

Determination of Parameters for Chaos in Dynamical Systems

It has been established that certain dynamical systems go into chaotic mode for some parameter values/ initial conditions. We have developed a computational framework which can be used to both explore the parameter space for points where the Lyapunov exponent is positive(implying chaotic behavior) and visualize the connections between parameters leading to these positive values. We demonstrate the effectiveness of the framework on several dynamical systems used to model bacterial populations with a nutrient source.

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PP1

Rapid Evaluation to Prevent Dangerous Regimens for An Artificial Pancreas Controller

The artificial pancreas (AP) controller presents one of the most promising treatment strategies for diabetes. In order for an AP controller to work effectively, it must evaluate timing and dose schedules for insulin in real-time. In this work, we determine a method to efficiently characterize all eigenvalues of the nonlinear two-delay glucose-insulin system and enable the rapid evaluation of dosing schedules for the AP controller by coupling the Gauss-Lucas theorem with the Lambert W function.

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PP1

A Dynamical Analysis of the Transitions to Bursting in Neuronal Cells

We study the occurrence and stability of rhythmic outcomes generated by multifunctional 4-cell circuits coupled with reciprocal inhibitory synapses. We examine how variations in the circuit connectivity and temporal properties of individual cells can affect the rhythmic outcomes. This research intends to reveal plausible mechanisms in the switch among gait patterns in quadrupeds triggered by an external drive. We will emphasize the generation of gaits in locomotion CPGs that do not burst endogenously in our models. We will note the optimal connectivity for production of multiple quadruped gaits, such as walking and hopping.

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PP1

Modeling Gun Ownership As a Social Disease

Gun violence is a leading cause of premature deaths in the US. The goal of this study is to better understand how different social conditions may impact gun-ownership rate. We use a SIR-type model that treats gun ownership like a contagious social disease. The model divides the population into three classes: non-susceptible, susceptible, and gun owners. The model is used to assess the effectiveness of different approaches in lowering gun-ownership rate.

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PP1

Approaches for Coherent X-Ray Diffraction Imaging of Paramecium Bursaria Chlorella Virus-1

Paramecium bursaria Chlorella virus-1 viruses exist in freshwater worldwide, and the outer capsid has been solved by cryo-EM method. We used Coherent X-ray diffractive imaging (CDI) to study inside of this virus. The CDI experiment was carried out at the Atomic, Molecular and Optics (AMO) end-station. In total, we had over 200,000 possible diffraction patterns were identified and processed. In the poster, we will present methods fro classification and reconstruction, as well as the results.

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PP1

Image-Based Structural Modeling of the Cardiac Purkinje Network

The Purkinje network plays an important role in the development and maintenance of cardiac arrhythmias; however, few modeling studies aim to develop structural models based on real physiological data. We present a method for creating three-dimensional Purkinje structural models based directly on imaging data in which Purkinje network structures extracted from photographs are projected onto realistic endocardial surfaces. The resultant models for the combined ventricle-Purkinje system have the potential to help elucidate Purkinje network contributions during ventricular arrhythmias.

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PP1

A Novel Approximation Method for Equilibrium Single-Channel Ca^{2+} Domains

A novel approximation for equilibrium Ca^{2+} and buffer concentrations near a single open Ca^{2+} channel is obtained by matching small- and large-distance behavior of the concentration functions. Compared to the widely-used rapid buffer and linearized approximations, the accuracy of the new method is uniform with respect to Ca^{2+}-buffer binding parameters. Although this method cannot be extended to multiple channels or buffers, it can be adapted to buffers with cooperative Ca^{2+} binding.

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PP1

Normal Forms and Unfoldings of Conductance-Based Neural Models

Conductance-based neural models are a class of ordinary differential equation systems derived from biophysical principles to describe the electrical dynamics of single neurons. We present the reduction of conductance-based models to normal forms, which are more analytically tractable. We also present unfoldings, treating bifurcation points as organizing centers, of conductance-based models, which make apparent their dynamic repertoire.

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PP1

Bidirectionality Induced by Cargo Thermal Fluctuations in Motor-Mediated Transport

We propose a model for bidirectional motor transport where direction switching is induced by cargo thermal fluctuations. Motivated by an Ornstein-Uhlenbeck-like process, we observe the slow response of motors to rapid fluctuations in the cargo. We construct a mean-field model of motor dynamics to establish the forces exerted. The resulting system is bistable, with two states corresponding to bidirectionality. The time to switch between directions is estimated using a weak noise approximation and WKB theory.

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PP1

Noise-Induced Switching in Stochastic Population Models

The study of systems with multiple metastable states is important to the field of ecology. Here we investigate cycling in stochastic population models. Methods from statistical mechanics are used to construct the optimal path to extinction. In addition, a probabilistic argument is used to understand the pre-extinction dynamics and approximate the mean time to extinction (MTE). Analytical results agree well with numerical Monte Carlo simulations. A control method is implemented to decrease the MTE.

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PP1

Review of Modeling of cAMP Action in Pancreatic Beta Cells

In pancreatic beta cells, cAMP is well known as being involved with the amplification factor pathway for insulin release. We have recently focused on describing spatial localization of catalytic protein kinase A in response to cAMP as well as how cAMP reflects the underlying metabolic dynamic in beta cells. In this presentation we review the impact modeling of cAMP has had on understanding beta cell dynamics and look to some open questions.

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PP1

Study of Viral Coinfection Dynamics in Human Respiratory Tract

Studies have found that 70% of hospitalized patients with influenza-like illness are infected with at least two different viruses, but no study has yet investigated the time course of these simultaneous infections in human respiratory tract. We use a mathematical model to study the dynamics of coinfection of respiratory tract to understand the severity, infectious period of coinfections. We are also interested to understand the viral dynamics considering cell regeneration, cellular coinfection in our model.

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PP1

Sensory Feedback in a Bump Attractor Model of Path Integration

Mammalian spatial navigation systems utilize several different sensory information channels. This information is converted into a neural code representing the animal's spatial position. In particular, spatial landmarks can be utilized to generate a more accurate representation of position, since velocity-integration alone can be error prone. Employing a bump attractor model, we explore how errors in path integration generated by synaptic heterogeneity and noise fluctuations can be corrected by feedback from positional cues.

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PP1

One-Dimensional Model of Blood Flow Discretized with Runge-Kutta Discontinuous Galerkin Methods

In this work we investigate a nonlinear hyperbolic system of conservation laws modeling one-dimensional blood flow through an elastic vessel. Solutions to this model are approximated using Runge-Kutta discontinuous Galerkin methods, and some convergence results are provided. We present numerical results for physiological networks of vessels modeling arterial and venous trees, with application to cardiovascular systems impacted by congenital heart defects and palliative surgeries.

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PP1

Mathematical Modeling of the Acute Inflammatory Response and Energy Consumption

When an external agent, such as a pathogen, enters the body, an acute inflammatory response is activated aiming to completely eliminate the invader. However, in some patients an overreaction of the immune system may occur which can lead to collateral tissue damage, organ failure and septic death. In the process of healing, energy is produced and consumed. In this work we developed a differential equations model to explore the role of Adenosine Triphosphate (ATP) and Nitric Oxide (NO) during an acute inflammatory response. We also studied the bifurcations that occur when we let certain parameters vary.

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PP1

Modeling Baroreflex Regulation of Blood Pressure and Heart Rate During the Valsalva Maneuver

The Valsalva Maneuver (VM) is the process of forceful exhalation against a closed airway. The VM has a shape that characterizes normal heart rate (HR) and blood pressure (BP) modulation in response to passive (breath-holding) and active (baroreflex control) effects. Deviation from the general shape of the graphs indicates significant issues with autonomic control. This study aims to use data from patients administered endotoxin to model diseased versus healthy states and to estimate parameters to fit the model.

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PP1

Redundancy, Degeneracy, and Robustness in Protein-Interaction Networks

To assess the impact of a drug on a biological system, network pharmacology uses impact measures that describe the effect of perturbations on networks. The plausibility of impact measures depends on their ability to capture the robustness of biological systems. The biological literature has highlighted links between redundancy, degeneracy, and

robustness. We investigate how to translate the biological notions of redundancy and degeneracy to network analysis by adapting an information-theoretic approach previously applied in neuroanatomy.

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PP1

A Model to Track Density and Average Mass of Brown Shrimp in Gulf of Mexico

Structured population models are used for modeling changes in the density of individuals over time and other factors such as age, mass, developmental stage and space. Mass is a particularly useful measure of condition of a population. Our approach to modeling mass dependent population dynamics introduces mass as an additional dependent variable. We develop a reaction diffusion-hyperbolic system of coupled nonlinear partial differential equations to track density and average mass of the population at location 'x' and time 't' and we apply it to brown shrimp population in gulf of mexico.

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PP1

Host-Pathogen Coevolution Generates Trade-Offs in Complexity Between the Level of the Cell Surface Receptor and the Gene Regulatory Network for Host Resistance

We integrate infectious disease dynamics with gene regulatory networks to study the evolution of host resistance to pathogens. We consider evolution at two levels: at the protein-protein interaction (PPI) level, pathogens coevolve with host receptors, while at the network level, hosts evolve expression changes for receptors. High complexity at the PPI level constrains host range, encouraging higher regulatory complexity, whereas lower PPI complexity expands host range and induces hosts to use PPI for resistance.

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PP1

Global Dynamics of a Mean Field Model of the Neocortex

We introduce a model for electroencephalographic activity in the neocortex as a system of coupled ODEs and PDEs. We present existence, uniqueness, and regularity of solutions, and conditions required on the phase space of the model for physiological plausibility of the evolution. We show the existence of bounded absorbing sets and address challenges toward establishing a global attractor theory. We point out how the presented results can be used in computational analysis of the model.

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PP1

Overcoming Chemotherapy Resistance by Inhibition of Mgmt and Apng in Glioblastoma Multiforme: A Mathematical Approach.

Patients diagnosed with glioblastoma are expected to survive only 14 months due to chemotherapy resistance. To overcome this, a new class of drugs is under development, which works by inhibiting DNA-repair enzymes. Developed in collaboration with experimentalists we present a mathematical model that simulates the treatment of glioblastoma with standard chemotherapy (Temozolamide) and the new drug. By incorporating detailed mechanisms of drug actions, we predict the potential for such treatment in improving patient survival times.

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PP1

Mathematical Modeling of Enzymatic Assays: Incorporating Experimental and Parametric Uncertainty

Blood coagulation is a complex network of biochemical reactions, many of which are mediated by enzymes. To assess the ability of blood to coagulate, e.g., monitoring anticoagulant treatments, the activity of enzymes must be tested experimentally. We seek a quantitative understanding of the uncertainty involved with such experiments. We use generalized polynomial chaos to model uncertainty due to experimental processes as well as kinetic parameters and quantify this dependence on our model.

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PP1

Abrupt Transitions from Low to High Firing Frequencies in Neurons and Neuronal Networks

What conditions lead to runaway activity in neuronal networks with recurrent excitation? We examine this question by analytically and numerically analyzing the parameters in the theta neuron with self-excitation, the LIF neuron with self-excitation and self-inhibition, the reduced Traub-Miles neuron with recurrent self-excitation, and the PING network model with NMDA and AMPA synapses. We find minimum requirements needed to create a "bump' mechanism whereby sudden transitions from low firing frequency to runaway activity can occur.

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PP1

Modeling the Distribution of Interspike Intervals of Spontaneous Activity in Afferent Neurons of the Zebrafish Lateral-Line

We have built stochastic models and analyzed the distribution of interspike interval (ISI) of spontaneous action potentials generated by afferent neuron in the absence of external stimuli, upon glutamate release by hair cells. In mammalian auditory system, ISI train shows negative correlation indicating synaptic depletion. In the zebrafish lateral line, the correlation is positive, possibly because synaptic connection is not one-to-one. We explore possible mechanisms of indirect coupling between hair cells.

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PP1

Asymptotic Phase for Stochastic Oscillators

The asymptotic phase of a limit cycle is a map from the basin of attraction to the circle, that has a uniform rate of change under the flow. The classical definition, for deterministic ODE systems, breaks down when the dynamics are stochastic. We show how to generalize the asymptotic phase for stochastic oscillators, as the complex argument of the eigenfunction associated with the slowest decaying complex eigenvalues of the adjoint Kolmogorov operator.

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PP1

Studying the Effects of Antiarrhythmic Drugs on Restitution Properties of Action Potential Duration of Human Ventricular Cells.

We investigate the effects of various antiarrhythmic drugs on restitution properties of action potential duration of ventricular cells by using a human ventricular cell model. The restitution hypothesis suggests that the slope of the restitution curve governs the transition to alternans. Our study examines the slope of these curves for different drugs to determine whether they are proarrhythmic or antiarrhythmic.

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PP1

Scroll Wave Filaments Pin to Various Objects

In three-dimensional reaction diffusion systems, excitation waves may form and rotate around a one-dimensional phase singularity called the filament. Filaments may pin to nonreactive objects, changing their behavior. We use numerical simulations to study how different configurations of such objects affect circular filaments. This work yields insights into the pinning of scroll waves in excitable tissue such as cardiac muscle, where scar tissue acts in a way similar to the nonreactive objects.

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PP1

Emergence of Longevity-Dependent Spatial Patterns in the Expression of a Small Heat Shock Protein

Spatial expression patterns of a small heat shock protein in *Caenorhabditis elegans* predict longevity following heat shock. We hypothesize these patterns are caused by reaction-diffusion processes of upstream molecules in the system. Specifically, insulin-like peptides diffuse from the head of the worm towards the tail and interact with DAF-2 receptors leading to activation or inhibition of the heat shock response. We will present the reaction-diffusion model that we developed to test this hypothesis.

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PP1

A PDE-ODE Model of Cell Polarization in Fission Yeast

We consider a one-dimensional PDE-ODE model of cell polarization in fission yeast. The model represents bulk diffusion of a signaling molecule in the cytoplasm, which is coupled to a pair of delay differential equations at the ends of the cell via boundary conditions. We investigate oscillatory solutions of the model as a function of cell length and diffusivity, and show how an asymmetric (polarized) solution switches to a symmetric (unpolarized) solution at a critical length.

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PP1

Numerical Methods for a 2D Convergent Reaction Diffusion Master Equation on Unstructured Mesh

Stochastic Reaction Diffusion Master Equations (RDMEs) have been widely used in biochemistry, computational biology, and biophysics to understand the reaction and diffusion of molecules within cells. However, the lattice RDME does not converge to any spatially-continuous model incorporating bimolecular reactions as the lattice spacing approaches zero. In order to contribute to a more accurate solution to this problem, this research aims to produce a 2D convergent RDME (CRDME) and efficient numerical methods for approximating its solutions. By considering the complex geometry of a real cellular domain, this research also aims to extend the methods to approximate the solution on unstructured meshes by implementing finite element method (FEM).

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PP1

Modeling Migration of the Zebrafish Posterior Lateral Line Primordium

The zebrafish lateral line is a sensory system that detects water movement patterns. The sensory organs that make up the lateral line are deposited by a migrating primordium during development. We develop chemotactic models of primordium migration and derive traveling wave solutions for CXCL12a and FGF, the ligands that guide primordium migration. Our model predicts primordium velocity as a function of length and shows that effective migration can only occur if ligand diffusion is limited.

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PP2

Minisymposterium: Soft Contact Lens Hydration Modeling

Excessive dehydration in contact lenses can lead to dry eye and discomfort for the wearer. Previous work in modeling the hydration levels in contact lenses has demonstrated the convergence of the hydration level to an oscillatory steady state with a fixed hydration gradient in the one-dimensional case. We present a simpler model, based on the heat equation, which reproduces this phenomenon and extend our model into two dimensions. Predictions on the gradient are shown.

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PP2

Minisymposterium: Tear Film Dynamics in Breakup with a Rough Ocular Surface

Tear breakup (TBU), a common symptom of dry eye syndrome, occurs when the tear film covering the ocular surface (OS) reaches a threshold minimum thickness. We model TBU with thin film equations, incorporating evaporation and OS roughness. We spatially discretize with Fourier spectral methods and solve the resulting DAE using backward differentiation methods. We find that the roughness visible in ophthalmological imaging is indeed the rough OS exposed by TBU.

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PP2

Minisymposterium: Tear Film Rupture Driven by Locally Elevated Evaporation Rates

Following recent studies by Peng et al. (2014), we investigate the influence of spatial variation in the tear-film lipid layer on the evaporation-driven tear-film rupture. While reductions in the lipid layer lead to locally elevated evaporation rates, the effects of healing flows driven by capillary forces and osmolarity also need to be considered. A simplified model is proposed to capture the key features of tear-film rupture and results are compared with the original model.

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PP2

Minisymposterium: On the Computation of the Wavefront After Contact Lens Motion

Contact lens motion can cause poor vision correction for patients with high visual aberrations. Unlike prior work, we consider contact lens motion to be a 3D rotation instead of 2D rotation and decentration. We present a technique for calculating the 3D rotation matrix using markers on the lens. We present a new method to determine the new wavefront after the lens has moved. This result will enable quantify errors in visual correction by contact lens.

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PP2

Minisymposterium: An Investigation of the Influence of a Blink on the Tear Film Dynamics

We simulate the tear film dynamics on a realistic blinking eye-shaped domain to examine the influence of the blink on the tear film formation. Using video of a blinking eye, we create a realistic moving eye-shaped domain by fitting the computational boundary curves to lid margins in the video. We then implement a moving overset grid method to numerically approximate a tear film model. Our results are compared with prior modeling results and experimental observations.

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PP2

Minisymposterium: Tear Film Dynamics: Modeling the Glycocalyx as a Poroelastic Region

The human tear film is a complex fluid structure composed of an aqueous layer, an outermost lipid layer, and the glycocalyx, a forest of large transmembrane mucins that provide stability to the ocular surface. We formulate a thin film model based on lubrication theory in order to understand the dynamics between the aqueous layer and the glycocalyx, which we treat as a poroelastic region.

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PP2

Minisymposterium: Tear Film Dynamics From a Flexible to a Rigid Blob Model

Tear film break up (TBU) occurs after imperfections in the lipid layer arise and cause elevated evaporation for large enough spots, but can also occur near blobs of lipids that are too small for the evaporative mechanism to account for the dynamics. We model the dynamics of the tear film beneath and near a blob with fixed surfactant concentration. We analyze how a transition from a flexible to rigid model blob affects tear film dynamics.

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PP3

Trafficking-Based Turing Mechanism for Pattern Formation on a Growing Domain

During development of C. elegans, the density of ventral cord synapses containing GLR-1 is kept constant despite significant changes in neurite length. We hypothesize an underlying Turing mechanism for synaptogenesis involving a short-range activator CAMKII, which moves via diffusion, and a long-range inhibitor GLR-1, which is trafficked along the ventral cord. We show that our novel trafficking-based mechanism supports Turing instabilities on a growing domain and the C. elegans system fits this paradigm.

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PP3

Identification of Significant Gene Via Unconventional Method in Gene Expression for Cancer Classification

A huge amount of data via high-throughput technology creates venue of learning and new research dimensions. However, most of the data undergo certain essential steps result in removal of data considered as noise (i.e. redundant and degeneracy). In this study, the significance of noise data was evaluated. And certain "significant genes' were identify that cast accuracy better than the normal ones found through statistical learning. Moreover, the results were tested against the normal practice conducted in machine learning for molecular classification of cancer.

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