SIAM.CSS2017
SIAM Central States Section 2017 Meeting

4 plenary talks, 25 mini-symposia, 4 posters

Plenary Talk
Numerical Homogenization and Multiscale Methods for Heterogeneous Problems
Yalchin Efendiev, Texas A&M University

In this talk, I will discuss multiscale model reduction techniques for problems in heterogeneous media. I will discuss homogenization-based multiscale methods and their relation to multiscale finite element methods. I will describe a general multiscale framework for constructing local (space-time) reduced order models for problems with multiple scales and high contrast. I will focus on a recently proposed method, Generalized Multiscale Finite Element Method, that systematically constructs local multiscale finite element basis functions on a coarse grid. I will discuss the issues related to the construction of multiscale basis functions, main ingredients of the method, and a number of applications. These methods are intended for multiscale problems without scale separation and high contrast.

Plenary Talk
A New Approach to Stochastic Inverse Problems for Scientific Inference
Don Estep, Colorado State University

The stochastic inverse problem for determining parameter values in a physics model from observational data on the output of the model forms the core of scientific inference and engineering design. We describe a recently developed formulation and solution method for stochastic inverse problems that is based on measure theory and a generalization of a contour map. In addition to a complete analytic and numerical theory, advantages of this approach include avoiding the introduction of ad hoc statistics models, unverifiable assumptions, and alterations of the model like regularization. We present a high-dimensional application to determination of parameter fields in storm surge models. We conclude with recent work on defining a notion of condition for stochastic inverse problems and the use in designing sets of optimal observable quantities.

Plenary Talk

Entropy Stable High Order Discontinuous Galerkin Methods for Hyperbolic Conservation Laws

Chi-Wang Shu, Brown University

It is well known that semi-discrete high order discontinuous Galerkin (DG) methods satisfy cell entropy inequalities for the square entropy for both scalar conservation laws and symmetric hyperbolic systems, in any space dimension and for any triangulations. However, this property holds only for the square entropy and the integrations in the DG methods must be exact. It is significantly more difficult to design DG methods to satisfy entropy inequalities for a non-square convex entropy, and / or when the integration is approximated by a numerical quadrature. In this talk, we report on our recent development of a unified framework for designing high order DG methods which will satisfy entropy inequalities for any given single convex entropy, through suitable numerical quadrature which is specific to this given entropy. Our framework applies from one-dimensional scalar cases all the way to multi-dimensional systems of conservation laws. For the one-dimensional case, our numerical quadrature is based on the methodology established in the literature, with the main ingredients being summation-by-parts (SBP) operators derived from Legendre Gauss-Lobatto quadrature, the entropy stable flux within elements, and the entropy stable flux at element interfaces. We then generalize the scheme to two-dimensional triangular meshes by constructing SBP operators on triangles based on a special quadrature rule. A local discontinuous Galerkin (LDG) type treatment is also incorporated to achieve the generalization to convection-diffusion equations. Numerical experiments will be reported to validate the accuracy and shock capturing efficacy of these entropy stable DG methods. This is a joint work with Tianheng Chen.

Plenary Talk

Topology-based Deep Learning for Drug Discovery

Guowei Wei, Michigan State University

Designing efficient drugs for curing diseases is of essential importance for the 21st century's life science. It involves an extremely complicated procedure, including disease identification, target hypothesis, virtual screening, drug structural optimization, preclinical in vitro and in vivo tests, clinical trials and finally optimizing drug's efficacy, toxicity, and pharmacokinetics properties. We integrate algebraic topology and deep learning algorithms for high throughput drug screening and design, including the predictions of drug binding poses, binding affinity, solubility, partition coefficient, and toxicity. We demonstrate that the proposed mathematical strategies outperform other conventional methods.

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MS01 "Tools for Efficient Forward, Inverse, and Stochastic Models"

Mahadevan Ganesh, Colorado School of Mines, mganesh@mines.edu

Photoacoustic Tomography and Thermodynamic Attenuation

Sebastian Acosta, Texas Children's Hospital, sacosta@bcm.edu

We consider a mathematical model for photoacoustic imaging to take into account attenuation due to thermodynamic dissipation. The propagation of acoustic waves, governed by a scalar wave equation, is coupled to the heat equation for the excess temperature due to the thermal expansivity of the medium. For photoacoustic tomography, we seek to recover the initial acoustic profile from knowledge of acoustic boundary measurements. From the theoretical point of view, we investigate whether the thermodynamic coupling affects the uniqueness/stability of the reconstruction. This inverse problem is a special case of boundary observability for a thermoelastic system. This leads to the use of control/observability tools to prove the unique and stable recovery of the initial acoustic profile in the weak thermoelastic coupling regime. We will discuss theoretical challenges in the strong coupling regime. We also propose and implement (numerically) a reconstruction algorithm. We will discuss numerical challenges associated with this implementation and opportunities for collaboration.

Ultra-efficient Reduced Basis Method and Its Integration with Uncertainty Quantification

Yanlai Chen, UMass Dartmouth, yanlai.chen@umassd.edu

Models of reduced computational complexity is indispensable in scenarios where a large number of numerical solutions to a parametrized problem are desired in a fast/real-time fashion. Thanks to an offline-online procedure and the recognition that the parameter-induced solution manifolds can be well approximated by finite-dimensional spaces, reduced basis method (RBM) and reduced collocation method (RCM) can improve efficiency by several orders of magnitudes. The accuracy of the RBM solution is maintained through a rigorous a posteriori error estimator whose efficient development is critical and involves fast eigensolves. After giving a brief introduction of the RBM/RCM, this talk will show our recent work on significantly delaying the curse of dimensionality for uncertainty quantification, and new fast algorithms for speeding up the offline portion of the RBM/RCM by around 6-fold.

A Class of Efficient Forward and Inverse 3D Dielectric Media UQ Models

Mahadevan Ganesh, Colorado School of Mines, mganesh@mines.edu

We consider electromagnetic wave propagation in three dimensional (3D) unbounded dielectric media governed by the Maxwell partial differential equations (PDE), radiation and interface conditions. The piecewise constant PDE coefficients are such that the continuous PDE model is well-posed for all frequencies, and as the frequency tends to zero, the electric and magnetic fields uncouple gracefully. The corresponding equivalent surface integral equation formulation and analysis open problem was solved recently by the author and his collaborators (Hawkins and Volkov). Using the robust continuous formulation, we develop a class of efficient associated discrete forward and inverse uncertainty quantization models.

Highly Accurate Equation Based Finite Difference Method Coupled with Farfield ABC for Acoustic Scattering

Dane Grundvig, Brigham Young University, danesvig@gmail.com

A fourth order finite difference method for time-harmonic acoustic scattering in polar coordinates is obtained. We adopt the equation based approach in the interior of the computational domain combined with a high order farfield expansion ABC (FFE-ABC). This consists of adding the fourth order terms of the truncation error to a standard second order method and then using the Helmholtz equation to reduce the order of the derivatives present in the truncation error. At the artificial boundary of the farfield expansion ABC, the application of the equation based

approach is very convenient due to the semi-explicit nature of the FFEABC. This technique renders a 9-point numerical scheme in the interior which is no wider in any coordinate direction than the standard second order scheme. We perform numerical experiments for Dirichlet BVPs that leads to the fourth order convergence of the numerical solution. Comparison with alternative fourth and sixth order methods reveals the high accuracy of this method.

Structure-preserving Exponential Integrators for Damped-driven PDE
Brian Moore, University of Central Florida, brian.moore@ucf.edu

Many PDE models for nonlinear waves have conservative properties (such as energy, momentum, mass, etc.) which are desirable to preserve in numerical simulations. In the presence of a driving force or damping terms those conservative properties inevitably break down. Yet, in cases where the forcing and/or damping is linear, with coefficients that depend on time, those properties may be preserved through discretization using exponential integrators. Various methods are developed generally, and damped-driven NLS equations are used to demonstrate the results.

Toward Optimal Recovery of Compressible Orthogonal Expansions
Akil Narayan, University of Utah, akil@sci.utah.edu

Many models that are parameterized by a finite number of random variables can be understood or analyzed by approximating the parametric dependence via a linear expansion in basis elements. When the random variable is high-dimensional, one is often interested in computation of expansion coefficients that are sparse or compressible. We propose and discuss a novel sampling and weighting scheme for the approximation of sparse or compressible expansions in a multivariate orthogonal basis. When the basis stems from a tensorial measure, the proposed method has uniform near-optimal recovery properties. The algorithmic procedure involves sampling from measures that are "induced" by univariate measures. We present recovery examples for a variety of tensorial measures and basis sets that showcase the efficacy of the procedure in both low- and high-dimensional problems.

Waves in Random Media: Asymptotics and Applications
Oliver Pinaud, Colorado State University, pinaud@math.colostate.edu

The motivation for this work is the reconstruction of inclusions in complex media. The fine structure of the medium of propagation is here not available and is thus modeled as random. When the fluctuations are too strong, this precludes the use of standard imaging techniques that are based on the complete knowledge of the medium. We propose an alternative based on deterministic transport models that describe the propagation of the average of weakly random quadratic quantities in the wavefield. The crucial part of the approach is to quantify the error made by approximating weakly random processes by their average. Media with short-range and long-range correlations are considered and numerical simulations validating the theory will be presented.

An FEM-MLMC Algorithm for a Class of Time-Dependent Stochastic Models
Brandon Reyes, Colorado School of Mines, breyes@mymail.mines.edu

We consider a class of time evolutionary models, comprising both deterministic and uncertain input data. We first develop an efficient finite element method (FEM) algorithm for the model for known input data. Subsequently we develop a stochastic multilevel Monte Carlo (MLMC)algorithm for the stochastic model. Our numerical experiments validate the efficiency of the FEM-MLMC model to compute stochastic moments for a physical quantity of interest in the model.

Optimal Low-rank Approximations of Bayesian Linear Inverse Problems
Alessio Spantini, MIT, spantini@mit.edu

In this talk we present statistically optimal and computationally efficient dimensionality reduction techniques for large-scale linear Gaussian inverse problems. These approximations of the Gaussian posterior distribution are at the heart of many state-of-the-art algorithms for nonlinear Bayesian inference. In particular, we study structure-exploiting approximations of the posterior covariance matrix as a low-rank update of the prior covariance matrix and prove optimality of the low-rank update for various metrics. These approximations are particularly useful when the data are informative relative to the prior only about a low-dimensional subspace of the parameter space. We also propose fast optimal approximations of the posterior mean that are particularly useful when repeated posterior mean evaluations are required for multiple sets of data (e.g., online inference). We extend these optimal approximations to the important case of goal-oriented inference where the quantity of interest (QOI) is a linear function of the inference parameters. We show that the posterior distribution of the QOI can be computed avoiding the explicit characterization of the full posterior distribution of the parameters. In particular, we focus on directions in the parameter space that are informed by the data, relative to the prior, and that are relevant to the QoI. This is joint work with Antti Solonen, Tiangang Cui, James Martin, Karen Willcox, Luis Tenorio and Youssef Marzouk.

Stochastic Tools for Large Linear Least-Squares and Inverse Problems
Luis Tenorio, Colorado School of Mines, ltenorio@mines.edu

I will briefly summarize properties of discrete quasimartingales (i.e., integrable, adapted processes on discrete time) that are useful for proving consistency of stochastic algorithms such asstochastic Newton and stochastic quasi-Newton approaches. These methods can be used to solve large linear least-squares and inverse problems where the large data sets present a significant computational burden (e.g., the size may exceed computer memory or data are collected in real-time). In the proposed framework, stochasticity is introduced in two different frameworks as a means to overcome these computational limitations.

Deferred-corrections Fourth and Sixth Order Schemes for Time-Harmonic Acoustic Waves
Vianey Villamizar, Brigham Young University, vianey@mathematics.byu.edu

In this paper we derive numerical methods to obtain numerical solutions with high order convergence to the exact solution of the scattering of acoustic waves. We base our derivation on the author's recently developed high order local Farfield Expansion absorbing boundary condition (ABC) [J. Comput. Phys. 333: 331-351,2017]. We exploit the property of the Farfield Expansion ABC to couple with any interior high order method and produce a new method with an overall order of convergence equal to the method employed in the interior. For the interior scheme, we use a deferred-corrections technique. As a result, we obtain numerical solutions approximating the exact solution which exhibit sixth and fourth order convergence, while employing the same 5-point stencil of the standard centered second order method. Numerical experiments for both Dirichlet and Neumann problems are performed and their results in terms of complexity, computational cost, and convergence are analyzed.

A Stochastic Approach to Reconstruction of Faults in Elastic Half Space
Darko Volkov, Worcester Polytechnic Institute, darko@wpi.edu

We introduce an algorithm for the simultaneous reconstruction of faults and slip fields on those faults. The physics of this problem are modeled using the equations of linear elasticity. We introduce a regularized functional to be minimized for the reconstruction. We prove that the minimum of that functional converges to the unique solution of the related fault inverse problem. Due to inherent uncertainties in measurements, rather than seeking a deterministic solution to the fault inverse problem, we consider a Bayesian approach. The advantage of such an approach is that we obtain a way of quantifying uncertainties as part of our final answer. On the downside, this Bayesian approach leads to a very large computation. To contend with the size of this computation we developed an algorithm for the numerical solution to the stochastic minimization problem which can be easily implemented on a parallel multi-core platform and we discuss techniques to save on computational time. After showing how this algorithm performs on simulated data and assessing the effect of noise, we apply it to measured data. The data was recorded during a slow slip event in Guerrero, Mexico.

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MS02 "Perspectives on Uncertainty Quantification"

Jehanzeb Chaudhry, University of New Mexico, jehanzeb@unm.edu
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Optimal Experimental Design Using Sampled Singular Values

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In modeling of physical systems, we often consider two types of quantities of interest (QoI): (i) observable QoI, and (ii) predicted QoI. We often use data associated with observable QoI to formulate and solve a stochastic inverse problem in order to quantify uncertainties in model inputs. Subsequently, these uncertainties may be propagated forward by the model in order to quantify uncertainties in the predicted QoI. However, when limited resources exist for gathering data on observable QoI, we are often tasked with determining the vector-valued observable QoI map for which we can collect data with available resources. We refer to choosing the QoI map as an experimental design. In this talk, we consider several design criteria based on sampling singular values of Jacobians to potential QoI maps to define various optimal experimental design problems. The approach presented does not require the specification of a prior density nor a description of the specific stochastic inverse problem to be solved. Numerical examples are used to illustrate the various concepts throughout the talk including discussion of an optimal experimental design problem involving the optimal configuration of buoys in Bay St. Louis to record maximum water elevations based on simulations of Hurricane Gustav (2008).

A Posteriori Analysis for Multi-step and Multi-stage IMEX Methods

Jehanzeb Chaudhry, University of New Mexico, jehanzeb@unm.edu

Implicit Explicit (IMEX) schemes are an important and widely used class of time integration methods for both parabolic and hyperbolic partial differential equations. We develop accurate a posteriori error estimates for a user-defined quantity of interest for multi-step and multi-stage IMEX schemes. The analysis proceeds by recasting the IMEX schemes into a variational form suitable for a posteriori error analysis employing adjoint problems and computable residuals. The a posteriori estimates quantify distinct contributions from various aspects of the spatial and temporal discretizations, and can be used to evaluate discretization choices. Numerical results are presented that demonstrate the accuracy of the estimates for a representative set of problems.

Towards Parallel in Time for Full Space Optimization

Eric Cyr, Sandia National Laboratories, eccyr@sandia.gov

Transient PDE constrained optimization is challenging due to repeated forward and backward transient simulation. When a simulation uses a spatial decomposition near the strong scaling limit, the time to solution for the optimization problem cannot be decreased by adding more computational resources. Addressing this issue requires algorithmic advancement in optimization algorithms and solution methods. This talk proposes a new parallel in time preconditioner for solving transient KKT systems arising in an inexact SQP algorithm. Our composite-step SQP algorithm utilizes inexact iterative solution of "benign" KKT systems, corresponding to a sequence of strictly convex quadratic programs. Its inexactness-handling mechanisms ensure global and fast local convergence. The preconditioner used to solve the KKT system is critical to the efficiency of this algorithm. Our preconditioner explicitly exposes continuity in time constraints using a time domain decomposition technique. These constraints are relaxed and the coupled forward-adjoint system is solved using a multigrid in time process. This talk will present the preconditoner and show results in a serial prototype indicating convergence independent of the number of time steps. The mesh independence of the preconditioner is demonstrated both standalone and when used within a Burgers equation constrained optimization problem.

Petrov-Galerkin FEM for Solving Second-order IVPs and its a Posteriori Error Estimation
Victor Ginting, University of Wyoming, vginting@uwyo.edu

We present a Petrov-Galerkin FEM for solving second-order IVPs from which a class of time integration schemes can be derived. Several standard techniques can also be recovered from this variational setting. The key in the derivation is the choice of finite element spaces and the numerical integration techniques utilized to calculate the functional in the variational equation. We discuss an adjoint-based a posteriori error estimate of the approximation. Several numerical examples are given to illustrate the performance of the resulting schemes and the corresponding error estimate.

Data-driven Polynomial Ridge Approximation Using Variable Projection
Jeffrey Hokanson, University of Colorado, jeffrey@hokanson.us

Inexpensive surrogates are useful for reducing the cost of science and engineering studies with large-scale computational models that contain many input parameters. A ridge approximation is a surrogate distinguished by its model form: namely, a nonlinear function of a few linear combinations of the input parameters. Parameter studies (e.g., optimization or uncertainty quantification) with ridge approximations can exploit its low-dimensional structure by working on the coordinates of the subspace defined by the linear combination weights, reducing the effective dimension. We introduce a new, fast algorithm for constructing a least-squares-fit polynomial ridge approximation from function samples. Naively, this would require optimizing both the polynomial coefficients and the subspace. However, given a fixed subspace the optimal polynomial coefficients solve a linear least-squares problem. Our proposed method exploits this structure by implicitly computing these coefficients using variable projection, which leaves an optimization problem over the subspace alone. We present an algorithm that finds the optimal subspace by optimizing over the Grassmann manifold using a Gauss-Newton Hessian approximation. We provide the details of the optimization algorithm, and we demonstrate its performance on several numerical examples. The Gauss-Newton method has superior theoretical guarantees and faster convergence than an alternating heuristic for ridge approximation proposed by Constantine, Eftekhari, and Ward [arXiv 1606.01929] that (i) optimizes the polynomial coefficients given the subspace and (ii) optimizes the subspace given the coefficients.

Quantification of Uncertainties for the Numerical Simulation of Compressible Multiphase Flows
Tulin Kaman, University of Arkansas, tkaman@uark.edu

Quantifying the uncertainties in the simulation of complex engineered systems is of considerable interest in a variety of science and engineering applications. It is essential to characterize and quantify the initial conditions effects in multiphysics, multiscale simulations to ensure the correctness of the computations. In recent years, there has been extensive research in modeling and developing numerical methods for compressible multiphase flows with the goal of better understanding the dynamics of flows that are involved in applications dealing with high explosives, solid alloys and propellants. The direct numerical simulation method for bubbly flows, based on the front tracking technique, has been used to study the dynamics of bubbles and interfaces as well as the propagation of shock waves in multiphase flows. The question regarding the roles of the initial conditions in the quantities of interest such as peak pressure and velocity is studied by performing efficient simulations (using the FronTier Multiphysics simulation package) on the number three supercomputer in the TOP500 list, Piz Daint.

Convergence of Distributions Arising from a Fixed Point Iteration
Simon Tavener, Colorado State University, simon.tavener@colostate.edu

Operator decomposition approaches for complex multiscale systems constitute an important class of inherently iterative solution procedures. When both stochastic and deterministic processes are present, additional complications arise. We consider a very general system of equations $ g(\lambda, u)=0, \, \lambda \in D \subset \mathbb{R}^d, \, u \in \mathbb{R}^n $, where $ \lambda $ is a single realization of a random variable Λ and the solution $ U=G(\Lambda) $ is also a random variable. We assume that the solution $ G(\lambda) $ must be obtained via an iterative (fixed point) procedure and address the convergence of \emph{distributions} of solutions U or of a quantity of interest $ q(U) $.

A Consistent Bayesian Approach for Stochastic Inverse Problems

Tim Wildey, Sandia National Labs, tmwilde@sandia.gov

Uncertainty is ubiquitous in computational science and engineering. Often, parameters of interest cannot be measured directly and must be inferred from observable data. The mapping between these parameters and the measureable data is often referred to as the forward model and the goal is to use the forward model to gain knowledge about the parameters given the observations on the data. Bayesian inference is the most common approach for incorporating stochastic data into probabilistic descriptions of the input parameters. We have recently developed an alternative Bayesian solution to the stochastic inverse problem based on the measure-theoretic principles. We prove that this approach, which we call consistent Bayesian inference, produces a posterior distribution that is consistent in the sense that the push-forward probability density of the posterior through the model will match the distribution on the observable data, i.e., the posterior is consistent with the model and the data. Our approach only requires approximating the push forward probability measure/density of the prior through the computational model, which is fundamentally a forward propagation of uncertainty. Numerical results will be presented to highlight various aspects of this consistent Bayesian approach and to compare with the standard Bayesian formulation.

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MS03 "Molecular Bioscience and Biophysics: Modeling and Computation"

Shan Zhao, University of Alabama, szhao@ua.edu
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Persistent Homology and Machine Learning for Structure-Based Biomolecular Property Predictions

Zixuan Cang, Michigan State University, cangzixu@math.msu.edu

The computational prediction of biomolecular properties is important in many applications such as protein design and drug discovery. Machine learning and deep learning have shown their power in describing target quantities for different objects, given sufficient datasets. With the fast growing biomolecular databases, we apply machine learning and deep learning methods for the structure-based prediction of biomolecular properties. We use persistent homology as a translator to provide descriptions of biomolecules suitable for machine learning algorithms. This topological method reduces geometric complexity, addresses the challenge of macromolecules, and delivers structured features while retaining the biological information. In this talk, I will describe the general pipeline for this approach and some applications, such as mutation induced protein stability change, protein-ligand binding affinity prediction, and virtual screening.

Fractional Poisson-Nernst-Planck Model for Ion Channels

Duan Chen, University of North Carolina at Charlotte, dchen10@uncc.edu

In this work, we propose a fractional Poisson-Nernst-Planck model to describe ion permeation in gated ion channels. Due to the intrinsic conformational changes, crowdedness in narrow channel pores, binding and trapping introduced by functional units of channel proteins, ionic transport in the channel exhibits a power-law-like anomalous diffusion dynamics. We start from continuous time random walk model for a single ion, and use a long-tailed density distribution function for the particle jump waiting time, to derive the fractional Fokker-Planck equation. Then it is generalized to the macroscopic fractional Poisson-Nernst-Planck model for ionic concentrations. Necessary computational algorithms are designed to implement numerical simulations for the proposed model and the dynamics of gating current is investigated. Numerical simulations show that the fractional PNP model provides a more qualitatively reasonable match to the profile of gating currents from experimental observations. Meanwhile, the proposed model motivates new challenges in terms of mathematical modeling and computation.

Bilayers as Local Structures of the Functionalized Cahn-Hilliard Functional

Shibin Dai, University of Alabama, sdai4@ua.edu

The functionalized Cahn-Hilliard (FCH) functional is a phenomenological model for the free energy of amphiphilic mixtures. We will talk about the variational properties of the FCH functional. It turns out that bilayers, filaments, and micelles are stable structures under energetically and geometrically localized perturbations.

Mathematical Models of Membrane Bending: Atomistic to Continuum

Michael Grabe, University of California at San Francisco, michael.grabe@ucsf.edu

In this talk I will describe recent advances we have made in using fast, continuum elasticity theory to describe membrane deformations around proteins. I will show that our calculations match the deformations predicted from all atom molecular dynamics simulations for two proteins: gramicidin (a small antibiotic ion channel) and nhTMEM16 (a member of the calcium activated chloride channel family). Our calculations reveal that nhTMEM16 produces large distortions in the membrane potentially related to its ability to scramble lipids from one leaflet to the other. This hypothesis is supported by atomistic simulations in which we observe lipids flipping from one leaflet to the other. Experiments to test the lipid flipping mechanism in a mammalian TMEM16 family member will also be discussed.

Data-driven Approach for Uncertainty Quantification with High Dimensional Random Space
Huan Lei, Pacific Northwest National Laboratory, huan.lei@pnnl.gov

Due to thermal fluctuation, biomolecule system exhibits high dimensional complex conformation space, where the explicit formulation of the underlying randomness is unknown in general. Traditional approaches show limitations to quantify the uncertainty propagation associated with such systems. We develop a data-driven approach to accurately construct the surrogate model for the quantify of interest, which is irrespective of the dependency and the analytical form of the underlying distribution. Our method is demonstrated in quantifying the uncertainty of the solvation energy of biomolecules modeled by Poisson-Boltzmann equation, and can be generalized to other systems with high dimensional arbitrary random space.

Wrinkling Dynamics of a Vesicle in Stokes Flow
Shuwang Li, Illinois Institute of Technology, sli@math.iit.edu

In this talk, we discuss 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 extension 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.

An Energy-preserving Scheme for PNP Equations
Xiaofan Li, Illinois Institute of Technology, lix@iit.edu

In this talk, we present a finite difference scheme that satisfies the energy dissipation law of the Poisson-Nernst-Planck equation exactly. We formulate the chemical potential differently and show that the energy-preserving scheme comes out of the new formulation. Numerical results comparing the energy-preserving scheme with the standard scheme will be shown.

Rigidity Strengthening: A Mechanism for Protein-Çoligand Binding
Duc Nguyen, Michigan State University, ddnguyen@math.msu.edu

Protein-coligand binding is essential to almost all life processes. The understanding of protein-coligand interactions is fundamentally important to rational drug and protein design. Based on large scale data sets, we show that protein rigidity strengthening or flexibility reduction is a mechanism in protein-coligand binding. It is found that the present approach outperforms all other state-of-the-art scoring functions for protein-coligand binding affinity predictions of two benchmark test sets.

Mathematics in Crime
Bao Wang, University of California at Los Angeles, wangbaonj@gmail.com

In this talk, I will speak about two aspects of mathematical modeling of crimes. One is how to mining spatial temporal sparse data. The other is how AI can be used for crime control. Our methods are generic, which can be applied to many other fields as well.

Multiscale Virtual Particle Based Elastic Network Model for Biomolecular Dynamic Analysis
Kelin Xia, Nanyang Technological University, xiakelin@ntu.edu.sg

In this talk, I will present the multiscale virtual particle based elastic network model (MVP-ENM). The multiscale virtual particle model is proposed for the discretization of biomolecular density data in different scales. Essentially, the model works as the coarse-graining of the biomolecular structure, so that a delicate balance between biomolecular geometric representation and computational cost can be achieved. To form ``connections" between these multiscale virtual particles, a new harmonic potential function, which considers the influence from both mass distributions and distance relations, is adopted between any two virtual particles. Unlike the previous ENMs that use a constant spring constant, a particle-dependent spring parameter is used in MVP-ENM. Two independent models, i.e., multiscale virtual particle based Gaussian network model (MVP-GNM) and multiscale virtual particle based anisotropic network model (MVP-ANM), are proposed. Even with a rather coarse grid and a low resolution, the MVP-GNM is able to predict the Debye-Waller factors (B-factors) with considerable good accuracy. Similar properties have also been observed in MVP-ANM. More importantly, in B-factor predictions, the mismatch between the predicted results and experimental ones is predominantly from higher fluctuation regions. Further, it is found that MVP-ANM can deliver a very consistent low-frequency eigenmodes in various scales.

New Finite Element Iterative Methods for Solving a Nonuniform Ionic Size Modified Poisson-Boltzmann Equation

Dexuan Xie, University of Wisconsin-Milwaukee, dxie@uwm.edu

In this talk, I will report a nonuniform size modified Poisson-Boltzmann equation (nuSMPBE) for a protein in a solvent with multiple ionic species. SMPBE is constructed by a new electrostatic free energy functional and solution decomposition techniques. It is proved to have a unique solution, and the solution satisfies a system consisting of nonlinear algebraic equations and one Poisson dielectric interface problem. To solve it numerically, new finite element iterative schemes are developed. Furthermore, they are programmed in Python and Fortran as a software package for solving nuSMPBE, and numerically tested on a Born ball test model and a protein in a sodium chloride solution and a sodium chloride and potassium chloride solution. Numerical results confirm the convergence of the new iterative schemes, and demonstrate the high performance of the new software package.

Geometric Singular Approach to Steady-State Poisson-Nernst-Planck Systems with Local Excess Chemical Potentials: Competition Bet

Mingji Zhang, New Mexico Institute of Mining and Technology, mingji.zhang@nmt.edu

We analyze a one-dimensional steady-state Poisson-Nernst-Planck system for ionic flows through a membrane channel with fixed boundary ion concentrations and electric potentials. We consider three ion species, two positively charged and one negatively charged, and assume zero permanent charge. Bikerman's local hard-sphere potential that depends on ion concentrations pointwise is included in the model to account for ion size effects. The model problem is treated as a boundary value problem of a singularly perturbed differential system. Our analysis is based on the geometric singular perturbation theory but, most importantly, on specific structures of this concrete model. The existence of solutions to the boundary value problem for small ion sizes is established and, treating the ion sizes as small parameters, we also derive an approximation of the individual flux and identify several critical potentials for ion size effects, from which qualitative properties of ionic flows are studied in great details.

A Two-Component Regularization for Charge Singularity in Implicit Solvation

Shan Zhao, University of Alabama, szhao@ua.edu

In this talk, we will present a new regularization method for treating charge singularity in solvated biomolecules whose electrostatics are described by the Poisson-Boltzmann (PB) equation. In a regularization method, by decomposing the potential function into two or three components, the singular component can be analytically represented by the Green's function, while other components possess a higher regularity. Our new regularization combines the efficiency of two-component schemes with the accuracy of the three-component schemes. Based on this regularization, a new matched interface and boundary (MIB) finite difference algorithm is developed for solving both linear and nonlinear PB equations. Compared with the existing MIB PB solver based on a three-component regularization, the present algorithm is simpler, easier to implement, and faster, while maintains the same second order accuracy. This is numerically verified by calculating the electrostatic potential and solvation energy on the Kirkwood sphere and a series of proteins. This is a joint work with Weihua Geng (Southern Methodist).

Rotational Diffusion of Membrane Proteins and Their Curvature Modulation

Yongcheng Zhou, Colorado State University, yzhou@math.colostate.edu

Some of the essential protein-carved membrane morphologies can't be characterized by individual mean curvature or Gaussian curvature. Orientational distribution of proteins turns out to be the controlling factor of the process, but was missing in most previous mathematical investigations. Here we use adopt the Onsager's variational principle to derive a Smoluchowski equation for the rotational diffusion of membrane proteins. This allows us to introduce the principle directions of proteins and membranes to the PDE, and further enables us to characterize the variation of orientations of proteins as they modulate/fit the dynamic membrane morphology.

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MS04 “Recent Advances in Computational Plasma Physics”

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A High Order Conservative Semi-Lagrangian Discontinuous Galerkin Method for the Vlasov-Poisson Simulations

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In this talk, we will introduce a high order conservative semi-Lagrangian (SL) discontinuous Galerkin (DG) method for the Vlasov-Poisson (VP) system. The proposed method relies on a characteristic Galerkin weak formulation and a high order characteristics tracing mechanism. Unlike many existing SL methods, the high order accuracy and mass conservation of the method are realized in a non-splitting manner. Thus, the detrimental splitting error, which could significantly contaminate long term Vlasov simulations, will be not incurred. One key ingredient in the scheme formulation is the use of Green's theorem which allows us to convert volume integrals into a set of line integrals. The resulting line integrals are much easier to approximate with high order accuracy, hence facilitating the implementation. The desired positivity-preserving property is further attained by incorporating a high order bound-preserving filter. To assess the numerical performance, we benchmark the proposed SLDG schemes for simulating several transport problems and the VP system. The efficiency and efficacy are numerically verified when compared with other prominent Vlasov solvers such as the Eulerian DG methods combined with Runge-Kutta time integrators.

Implicit Solution of the Vlasov-Poisson System

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Most Eulerian and semi-Lagrangian codes use a splitting in time approach for implicit, charged particle transport solvers. The reason for this is advection with respect to only position or only velocity can be solved explicitly and even exactly, but advection with respect to both position and velocity requires solving a linear system whose order is the size of the phase space discretization. This becomes unacceptable for higher dimensional problems. We propose a new approach which does not involve splitting in time, but splitting the phase space into subdomains. If each subdomain is appropriately chosen, the transport problem can be solved explicitly on each subdomain. A Krylov solver is then used to solve for the boundaries between subdomains, which involves a much smaller linear system than the one required for the no splitting approach.

High-Order Finite-Difference Time-Domain Methods for Electromagnetic Wave Propagation in Plasmonic Materials

Michael Jenkinson, Rensselaer Polytechnic Institute, jenkim2@rpi.edu

We propose new numerical schemes for the simulation of transient electromagnetic wave propagation in linear dispersive media where material properties are frequency dependent. Accurate time-domain simulations at interfaces between different dispersive materials are of particular interest in the fields of plasmonics and nano-photonics, with various applications in imaging, sensing, and computing. We formulate Maxwell's equations as a second-order wave equation with an additional term which is either a time-history integral or is coupled to an additional ODE. These formulations are modifications of the traditional recursive convolution and auxiliary differential equation approaches in the literature, and allow us to address material interfaces with complex curvilinear geometries, thereby avoiding the drawbacks of the well-known staggered Yee discretization. A modified equation time-stepping approach is used to obtain schemes of up to any desired order of accuracy. To preserve the accuracy at boundaries and interfaces, we use the physical interface and boundary conditions for Maxwell's equations to develop numerical compatibility conditions.

Positivity Limiters for Spectral Approximations of Linear Kinetic Transport Equations
Paul Laiu, Oak Ridge National Laboratory, laiump@ornl.gov

Kinetic transport equations describe the evolution of particle-based systems, such as rarefied gases, charged particles, and radiation. The kinetic description is given by a nonnegative scalar function of position, momentum, and time. Here we focus on the development and analysis of positivity limiters for spectral discretizations in the momentum variable. It is well-known that such discretizations may lead to negative particle concentrations in space, due to the fact that the underlying approximation is not always positive at the kinetic level. Standard positivity limiters address this issue by enforcing positivity of the spectral approximation on a finite set of preselected points. We consider several point-wise limiters of this type: some that have been proposed in different contexts and two that are new. We also present a new class of positivity limiters that impose weaker conditions on the spectral approximation and are therefore faster to compute. We give error estimates on the consistency for each limiter, run tests on a well-known benchmark problem, and compare the accuracy and efficiency of different limiters.

Asymptotic Preserving IMEX-LDG Schemes for Kinetic Transport Equations in a Diffusive Scaling
Zhichao Peng, Rensselaer Polytechnic Institute, pengz2@rpi.edu

We develop a family of high order asymptotic preserving (AP) local discontinuous Galerkin (LDG) schemes for kinetic transport equation in a diffusive scaling. Our approach is based on macro-micro decomposition and a reformulation of the decomposed system. With a proper application of globally stiffly accurate high order implicit-explicit Runge-Kutta (IMEX-RK) time integrator and a local discontinuous Galerkin spatial discretization, our scheme is unconditionally stable in the diffusive regime. In hyperbolic regime, our scheme has a time step restriction on the same level as the one for explicit upwind scheme solving transport equation. The limiting scheme is an implicit Runge-Kutta local discontinuous Galerkin scheme for the limiting equation. With energy analysis, we establish uniform stability and rigorously prove the AP property for schemes with first order IMEX-RK time integrator. Our scheme is implicit, but the underlying algebra system is sparse, positive definite and symmetric. The performance of the proposed schemes is demonstrated through a set of numerical examples.

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MS05 "PDEs in Fluid Dynamics: Analysis and Computations"

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Downscaling Data Assimilation Algorithm with Applications to Statistical Solutions

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Based on a down-scaling data assimilation algorithm, which employs a nudging term on the coarse scales, we construct a {\it determining map} of coarse scale trajectories and investigate its properties. This map is then used to develop a down-scaling data assimilation scheme for statistical solutions of the two-dimensional Navier-Stokes equations, where the coarse scale statistics of the system is obtained from measurements. As a corollary, we deduce that the statistical solutions for the Navier-Stokes equations are determined by their coarse mesh spatial distributions. This is based on a joint work with C. Foias, C. Mondaini and E. S. Titi.

Viscous Fluids in General Relativity

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We consider the problem of describing relativistic viscous fluids. More specifically, we study Einstein's equations coupled to a relativistic version of the Navier-Stokes equations. After motivating the problem and reviewing its history, we present recent results about well-posedness and causality of the equations of motion. If time allows, applications will be briefly discussed.

Geometry of 3D Turbulent Flows and the Scaling Gap in the 3D Navier Stokes Regularity Problem

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We show that the scaling gap in the 3D Navier-Stokes equation regularity problem can be reduced by an algebraic factor. All preexisting improvements have been logarithmic in nature, regardless of the functional set up utilized. This result is inspired by the geometry of the regions of intense vorticity observed in computational simulations of 3D turbulent flows.

Turbulence in Vertically Averaged 3D Rayleigh-Benard Convection

Michael Jolly, Indiana University, msjolly@indiana.edu

We look for features of 2D turbulence in the momentum equations that result from taking the vertical average of the 3D Rayleigh-Benard system. The 2D system has a body force which involves various integrals of the 3D flow. This force is time-dependent, and presumably in all modes. We extract 2D quantities from numerically computed solutions to the3D Rayleigh-Benard system to check the sharpness of rigorous bounds regarding 2D turbulence.

Analysis of a Stratified Kraichnan Flow

Davar Khoshnevisan, University of Utah, davar@math.utah.edu

We discuss some recent progress on the analysis of a special family of Kraichnan flows that describe the turbulent transport of a passive scalar quantity in a stratified, random velocity field. This is joint work with Jingyu Huang.

The Voigt Model as a Tool for Computationally Analyzing the Blow-Up of the 3D Euler Equations
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We report the results of a computational investigation of two recently proved blow-up criteria for the 3D incompressible Euler equations. These criteria are based on an inviscid regularization of the Euler equations known as the 3D Euler-Voigt equations. The latter are known to be globally well-posed. Moreover, simulations of the 3D Euler-Voigt equations also require less resolution than simulations of the 3D Euler equations for fixed values of the regularization parameter. Therefore, the new blow-up criteria allow one to gain information about possible singularity formation in the 3D Euler equations indirectly; namely, by simulating the better-behaved 3D Euler-Voigt equations. To test the robustness of the inviscid-regularization approach, we also investigate analogous criteria for blow-up of the 1D Burgers equation, where blow-up is well-known to occur.

Dynamics of Singularities, Wave-breaking and Turbulence in 2D Hydrodynamics with Free Surface
Pavel Lushnikov, University of New Mexico, plushnik@math.unm.edu

We consider 2D ideal fluid hydrodynamics free surface. A time-dependent conformal transformation maps free fluid surface in to the real line and fluid domain into the lower complex half-plane. Fluid dynamics is fully characterized by complex singularities in the upper complex half-plane of conformal map and complex velocity. Initially flat surface with the pole in the complex velocity turnsover arbitrary small time into the branch cut connecting two square root branch points. Lowest branch point approaches fluid surface with the exponential law corresponding to the formation of the fluid jet which produces wave breaking in the form of plunging of the jet into the water surface. The use of the additional conformal transformation to resolve the dynamics near branch points allows to analyze wave breaking in details. Formation of multiple Crapper capillary solutions is observed during overturning of the wave contributing to the turbulence of surface waves. Another way of wave breaking is the slow increase of Stokes wave amplitude through nonlinear interactions until the limiting Stokes wave forms with subsequent wave breaking. Square-root branch point is the only singularity in the physical sheet of Riemann surface for non-limiting Stokes wave. The corresponding branch cut defines the second sheet of Riemann surface after crossing the branch cut. The infinite number of square root singularities is found in the infinite number of non-physical sheets of Riemann surface. Increase of the steepness of the Stokes wave results in simultaneous approach of all singularities to the real line from different sheets of Riemann surface forming together 2/3 power law singularity of the limiting Stokes wave. It is found that non-limiting Stokes wave at the leading order consists of the infinite product of nested square root singularities which form the infinite number of sheets of Riemann surface. The conjecture is well supported by high precision simulations.

Continuous Data Assimilation for Miscible Displacement in Porous Media
Bradley McCaskill, University of Wyoming, bmccaski@uwyo.edu

We propose the use of a continuous data assimilation algorithm for miscible flow models in porous media. In the absence of initial conditions and concentration of the source term for the model, observed sparse measurements are used to generate an approximation to the true solution. Under certain assumption of the sparse measurements and their incorporation into the algorithm it can be shown that the resulting solution converges to the true solution at an exponential rate. Various numerical examples are considered in order to validate the convergence of the algorithm.

On the Convergence of Statistical Solutions of Evolution Equations
Cecilia Mondaini, Texas A&M University, cmondaini@math.tamu.edu

The concept of statistical solutions of evolution equations in fluid dynamics has emerged with the aim of proving rigorous results concerning the conventional theory of turbulence. For well-posed systems, a statistical solution corresponding to a given initial probability measure is trivially given by the transport of the initial measure by the semigroup. In this talk, I will present an abstract framework that allows one to prove the existence of such statistical solutions for evolution equations which are not known to be well-posed, by considering regularized approximate models. The aim is to show that the statistical solutions of the approximate models converge to a statistical solution of the original system. An application of this framework to the inviscid limit of the 2D incompressible Navier-Stokes equations will be discussed. This is a joint work with A. Bronzi and R. Rosa.

Data Assimilation in Geophysical and Fluid Dynamics
Yuan Pei, University of Nebraska-Lincoln, ypei4@unl.edu

We introduce some recent results on the continuous data assimilation algorithm in geophysical and fluid dynamics. In particular, we show the analysis of this algorithm for the two-dimensional magnetohydrodynamic equations, i.e., we prove that the interpolated solution converges to the reference solution in both L2 and H1 norms exponentially fast in time. Also, we present the numerical simulation of this algorithm and its improvement under the context of 1D Kuramoto-Sivashinsky equation. Part of the results is joint work with Animikh Biswas, Joshua Hudson, and Adam Larios.

Energy Stability of Hydrodynamic Systems Driven by a Stochastic Forcing
Jared Whitehead, Brigham Young University, whitehead@mathematics.byu.edu

Physically motivated convective systems have inherent noise that is in some cases well represented by an additional stochastic forcing. We consider two such cases wherein a bulk internal heat source is stochastic, and where the temperature boundary condition has an additive noise. Under certain realistic assumptions we compute a quasi-steady conductive solution to the system, and investigate the stability of the system about this conductive state using Monte-Carlo solutions of the corresponding eigenvalue problem. Future extensions of the technique will also be discussed.

Recent Developments on the Magnetohydrodynamics and Its Related Systems
Kazuo Yamazaki, University of Rochester, kyamazak@ur.rochester.edu

This talk discusses some recent developments on the magnetohydrodynamics (MHD) and related systems for both deterministic and stochastic perspectives. The equations of interest may include the MHD system, Navier-Stokes equations, micropolar and magneto-micropolar fluid systems, MHD-Hall system and Boussinesq system. The type of results to be discussed may include wellposedness and ergodicity, etc.

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MS06 "Numerical Simulation under Uncertainty"

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Sequential vs Joint Inversion of Probability Distributions

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We consider a problem of general interest in stochastic inverse problems involving the inversion of a distribution defined on the range of a parameter-to-observable map, and we use a disintegration theorem to describe the class of pullback measures solving this type of problem. Some numerical methods for constructing a particular pullback measure are discussed. Particular focus is given to drawing comparisons to the structure of solutions obtained iteratively through a "sequential" inversion that seeks to solve a sequence of lower-dimensional problems as opposed to solving a single higher-dimensional problem.

Statistical Analysis of Initial-condition Constraints and Parametric Sensitivity

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Experimental burns, such as the Fire and Smoke Model Evaluation Experiment (FASMEE), require careful preparation, including determining optimal sensor placement in the field to be studied, to improve coupled fire-weather simulations. Exploring the full uncertainty of such a high-dimensional problem, or even obtaining mean-state conditions, is not feasible. Instead, long records of measurements at selected weather stations are analyzed, to identify initial conditions that are somehow rigorously close to the long-term mean, conditioned on suitability for burns. Since the measured variables are physically and statistically incommensurate, close is defined by Mahalanobis distance: standardizing and decorrelating the mean-square distance to the mean, more heavily weighting distances along state-space directions with less variance. A large ensemble of coupled fire-atmosphere simulations is run for several key model parameters, including burn day, selected by Latin hypercube sampling. Sensitivity analysis is used to the isolate the variance of simulated measurements due to each parameter. Then, maps of variance and variance-fraction due to a parameter show locations where suitable measurements would improve that parameter. For more information, see http://tinyurl.com/y8ge2h9t.Work partially supported by Joint Fire Science Program grant 16-4-05-3.HPC (Yellowstone, Cheyenne supercomputers) was provided by NCAR, sponsored by the National Science Foundation.

Multi-grid and Multi-level Monte Carlo Method for Stokes-Darcy Model with Random Permeability

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Stokes-Darcy type models have attracted significant attention since it arises in many applications such as surface and subsurface flow interaction, groundwater flows in karst aquifers, petroleum extraction and industrial filtration. In the natural world, a lot of porous media has random permeability, especially in the subsurface flow system. We present multi-grid and multi-level Monte Carlo method for solving a stochastic Stokes-Darcy model with random permeability. Compared with the traditional Monte Carlo method, this method can significantly reduce the number of samples, hence improve the efficiency. Both theoretical and numerical results are presented to illustrate this method.

Functional Bayesian Data Assimilation with White Data Error Noise and Applications to Assimilation of Active Fires Satellite Set

Jan Mandel, University of Colorado at Denver, jan.mandel@ucdenver.edu

AVAST Spatial PDE-based models lead to Bayesian estimation of the state as a random smooth function. The posterior is ill-defined in general when both the state distribution and the data error distributions are Gaussian probability measures on an infinitely dimensional space. However, when the data error distribution is white noise, which is not a probability measure, the posterior is well defined as a probability measure, and we can prove large-sample convergence of the Ensemble Kalman filter in the linear case with randomization by white noise. More generally, data log likelihood defined by integration over the physical domain leads also to well-posted posterior distribution. As an application, we show assimilation of satellite active fires detection into a fire spread model. The state of the fire model is encoded as the fire arrival time, which is considered as a random smooth function on a spatial domain. A preconditioned steepest descent method can find a useful approximation of a maximum a posteriori probability estimate in one iteration, avoiding local maxima. Maximizing the data likelihood can be used to find the most likely ignition point and time automatically as well. This research was partially supported by NASA grant NNX13AH59G.

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MS07 "Advances in Anisotropic Mesh Adaption for Numerical Computations"

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Anisotropic Mesh Adaptation for Chan-Vese Image Segmentation Model

Karrar Abbas, University of Missouri-Kansas City, kka8cc@mail.umkc.edu

Chan-Vese variational model has been widely-used in image segmentation and provides good segmentation for different types of images including noisy images. On the other hand, most of the available implementations of the algorithm use finite difference method to solve the Euler-Lagrange equation of the energy functional (PDE model). In this study, we use finite element method to solve the PDE model with anisotropic mesh adaptation technique and compare the results with the ones obtained using finite difference method.

Anisotropic Mesh Adaptation for Porous Medium Equation in Fractured Reservoir

Ahmed Azeez, University of Missouri-Kansas City, amabp7@mail.umkc.edu

Porous Medium Equation (PME) is studied in fractured reservoir where permeability is much higher in fractures than that in matrix. Mesh adaptation around fractures is important in order to obtain accurate result efficiently. We review some commonly used mesh adaptation techniques and compare the results with our metric-based anisotropic mesh adaptation method. Numerical examples in 1D and 2D are presented.

Moving Simulation of Fourth Order PDES in 2D

Kelsey DiPietro, University of Notre Dame, kdipiet1@nd.edu

We develop a robust moving mesh finite difference method simulation of fourth order nonlinear PDEs describing elastic-electrostatic interactions in two dimensions. We use and extend the Parabolic Monge-Ampere methods developed by Budd and Williams to solve fourth order PDEs with varied evolutionary dynamics. The first PDE develops finite time quenching singularities at discrete spatial location(s). The moving mesh method must dynamically resolve the temporally forming singularities, all while preserving the underlying length scales of the problem. We show that the PMA resolves the singularities to high accuracy and gives strong evidence of self-similarity near blow up. The second PDE models a regularized system that considers elastic-electrostatic interactions after singularity occurs. The solution starts from an initially curved interface that propagates through the domain until it is pinned at the boundaries. In this case, the interface location and curvature characteristics are known from the beginning of the simulation, so the moving mesh method must dynamically shift points to track the interface and accommodate the growing interface perimeter. To accurately track the interface, we integrate the boundary layer analysis into the moving mesh PDE, resulting in greater resolution near all the boundary layers.

A New Functional for Variational Mesh Generation and Adaptation Based on Equidistribution and Alignment for Bulk Meshes

Avary Kolasinski, University of Kansas, avaryk@ku.edu

We will introduce a new meshing functional for variational mesh generation and adaptation with minimal parameters based on the equidistribution and alignment conditions. We will discuss the theoretical properties of this functional including its coercivity and the nonsingularity and existence of limiting meshes. We will then present a comparative numerical study of this new functional with one well known functional, which is also based on the equidistribution and alignment conditions. Finally, we will introduce the theory of variational mesh generation and adaptation on surface meshes.

Mesh Adaptation for Finite Element Solution of Anisotropic Porous Medium Equation
Xianping Li, University of Missouri-Kansas City, lixianp@umkc.edu

Anisotropic Porous Medium Equation (APME) is developed as an extension of the Porous Medium Equation (PME) for anisotropic porous media. A special analytical solution is derived for APME for time-independent diffusion. Anisotropic mesh adaptation for linear finite element solution of APME is discussed and numerical results for two dimensional examples are presented. The solution errors using anisotropic adaptive meshes show second order convergence.

Optimal Mass Transport-Based Approach for Anisotropic Adaptive Mesh Generation
Mohamed Sulman, Wright State University, mohamed.sulman@wright.edu

We consider generating anisotropic adaptive meshes based on solving the classical problem of the optimal mass transportation, also known as Monge-Kantorovich problem (MKP). The adaptive mesh is generated using a coordinate transformation that is computed as the unique solution of the optimal mass transport problem. The numerical solution of the MKP is obtained as the gradient of the steady state solution of a parabolic Monge-Ampre equation (PMAE). Several numerical experiments are conducted to demonstrate the performance of the PMAE method.

Adaptive Moving Mesh Central-Upwind Schemes for Hyperbolic System of Conservation and Balance Laws
Tong Wu, North Carolina State University, twu18@ncsu.edu

The development of accurate, efficient and robust numerical methods for the hyperbolic system of conservation/balance law is an important and challenging problem. One major numerical difficulty is related to the fact that the hyperbolic system admits non-smooth solutions. To achieve high resolution as well as to improve the efficiency of the numerical methods, we have developed new adaptive moving mesh (AMM) central-upwind schemes for the hyperbolic system of conservation/balance laws. The designed algorithm solves the PDE using the second-order semi-discrete central-upwind schemes and strong stability preserving Runge-Kutta ODE solver. After evolving the solutions to the new time level, the mesh points are then redistributed accordingly to the moving mesh PDE (MMPDE), together with a conservative projection strategy to project the solutions to the new mesh. We demonstrate the robustness and efficiency of AMM central-upwind schemes by a number of numerical examples of Euler equations of gas dynamics and the Saint-Venant system of shallow water equations for both 1-D and 2-D cases.

Selection of the Regularization Parameter in the Ambrosio-Tortorelli Approximation of the Mumford-Shah Functional for Image Segmentation.
Yufei Yu, University of Kansas, y920y782@ku.edu

Image segmentation is a process to find the boundary sets of a given image. In 1989, Mumford and Shah propose a functional whose minimization leads to optimal segmentation. However, the Mumford-Shah functional is inconvenient to carry out in practical computation due to its lack in regularity. Ambrosio and Tortorelli (1992) propose a phase-field regularization of the functional and show that it gamma-converges to the original functional as the regularization parameter goes to zero. On the other hand, in actual computation, people find that the regularization parameter has physical dimension and its choice can result in very different results. Even worse, the functional is found not to gamma-converge to the Mumford-Shah functional in some cases. In this talk we will present some theoretical explanations for this behavior. Moreover, we will present a strategy for choosing the regularization parameter for better segmentation effects. Numerical examples will be presented.

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MS08 "Applied Dynamical Systems"

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Iuliana Oprea, Colorado State University, juliana@math.colostate.edu
Gerhard Dangelmayr, Colorado State University, gerhard@math.colostate.edu

Virtually Defect-free Patterns and Undercompressive Shocks Produced by Ion Bombardment of Surfaces
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Bombarding a solid surface with a broad ion beam can yield a remarkable variety of self-assembled nanoscale patterns, including ripples and arrays of nanodots. The anisotropic Kuramoto-Sivashinsky (AKS) equation is widely used to model ripple formation induced by ion bombardment.The primary obstacle that has prevented the adoption of ion bombardment as a nano-fabrication tool is the high density of defects in the patterns that typically form. Our simulations indicate that this problem could be remedied simply by rocking the sample during ion bombardment. From a mathematical standpoint, we find that a temporally periodic coefficient in the AKS equation can suppress the spatiotemporal chaos characteristic of this equation and replace it with near perfect spatial periodicity. If a stationary sample is bombarded at near grazing incidence, experiments reveal phenomena that are not captured by the AKS equation. We have derived an equation of motion for the surface of an ion-bombarded material that differs from the AKS equation by the inclusion of a cubic nonlinearity. Our results establish that this term has a crucial influence on the dynamics --- it can lead to the formation of a terraced topography that coarsens in time, in accord with experimental observations. The rapid variations in the slope at the edges of the terraces are due to the formation of undercompressive shocks.

Regulatory Network Identification from Time Series Data
Bree Cummins, Montana State University, breecummins@gmail.com

Many molecular biology experiments are designed to track abundances of molecules over time with an eye to discovering molecular interactions. Given a time series data set, we seek the low dimensional regulatory networks among the measured molecules that best predict the experimental data. The key elements of our methodology are (a) dimension reduction of nodes in the network via domain knowledge and periodicity analysis; (b) dimension reduction of edges using optimization of parameters for a Hill function model; (c) construction and perturbation of putative networks from combinations of the reduced nodes and edges; and (d) comparison of network prediction of the data using discontinuous switching models of regulatory events. The talk will focus primarily on step (d), which is a method of analysis that applies to global parameter space rather than just to a select set of parameters. This is accomplished because switching systems permit a finite decomposition of parameter space such that within each region a coarse description of the trajectories in phase space remains constant. Trajectories from the experimental data set are either permissible or impermissible in each region of parameter space, and the number of parameter regions with permissible trajectories is a quantification of network performance in robustly reproducing the data.

On the Contribution of Phase Separation to Pattern Formation during Normal-Incidence Ion Bombardment of Binary Compounds
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We extend a model of Bradley and Shipman for the normal incidence ion bombardment of binary compounds to account for the effects of competing instabilities caused by the Bradley-Harper effect and ion-induced phase separation. Through a weakly nonlinear analysis and numerical integrations, we find that the phase difference between surface height and composition may serve as a useful indicator of which physical mechanism primarily contributes to the formation of experimentally observed ripples and nano-dot arrays. Our numerical simulations also suggest the existence of traveling wave solutions to our equations in the phase-separation regime.

Least Action Methods and Noise Induced Transitions in Periodically Forced Systems
John Gemmer, Wake Forest University, gemmerj@wfu.edu

We present a study of the metastability of periodic orbits for 1-D periodically forced systems perturbed by weak additive noise. It is well known that noise can introduce dramatic changes to the dynamics of the system, e.g. stochastic resonance, noise induced transitions between deterministic stable states etc. We ask the question: can noise induced transitions be completely understood using least-action principles and how do these results compare with classic results from large deviations? In particular, while pure noise induced transitions between metastable states occur on exponentially long time scales (Kramers rate) the frequency of the forcing introduces an additional time scale (inverse of the Floquet exponent) and a preferred phase of transition. Using least action principles, we show that the preferred phase and expected time of transition depend crucially on the scaling of these parameters.

Pattern Formation in the Wake of Growth Mechanisms
Ryan Goh, Boston University, rgoh@bu.edu

We study the effect of domain growth on the formation and selection of patterns. Domain growth is encoded in a step-like parameter dependence that allows patterns in a half plane, and suppresses them in the complement, while the boundary of the pattern-forming region propagates with fixed normal velocity. We study such fronts using rigorous techniques from dynamical systems and functional analysis, as well as continuation algorithms to explore solution sets numerically. In this talk we will discuss recent results in both one and two spatial dimensions in a variety of different pattern forming systems such as the Cahn-Hilliard, Complex Ginzburg-Landau, Swift-Hohenberg, and reaction-diffusion systems.

Where's Waldo? (and where isn't he): Neural Field Models of Memory-Guided Search
Zachary Kilpatrick, University of Colorado Boulder, zpkilpat@colorado.edu

Many organisms can remember locations they have already visited during a search. Experiments on visual search have shown exploration is guided away from the locations of previous visits, reducing the chance of scanning the same positions twice before finding the target. We develop and analyze a neural field model of the memory trace that directs exploration during search. The network consists of two coupled layers. A position-encoding layer sustains a localized activity bump corresponding to the searching agent's current location, and search is modeled by a velocity input that propagates the bump. A memory layer sustains persistent activity bounded by a wave front, whose edges are expanded in response to excitatory input from the position layer. Search is biased via inhibition-of-return due to the remembered locations, influencing directionality of subsequent velocity inputs. We use asymptotic techniques to reduce the dynamics of our model to equations that track the bump position and front boundary. Performance in target-finding tasks is then compared across different instantiations of the model. This is joint work with Daniel Poll at Northwestern University.

Optimizing Mixing in Laminar Flows: Aref's Blinking Vortex
James Meiss, University of Colorado at Boulder, jdm@colorado.edu

Mixing of a passive scalar in a fluid flow results from a two part process in which large gradients are first created by advection and then smoothed by diffusion. We will discuss methods of designing efficient stirrers to optimize the mixing of a passive scalar in a two-dimensional nonautonomous, incompressible flow over a finite time interval. The flow is modeled by a sequence of area-preserving maps whose parameters change in time, defining a mixing protocol. As an example, we study a version of Aref's blinking vortex flow; here the stirrers are modeled as point vortices. The position and strength of the vortices represent parameters to be selected to optimize the stirring efficiency. Stirring efficiency is measured by a version of a "mix-norm", a negative Sobolev seminorm; its decrease implies creation of fine-scale structure. A Perron-Frobenius operator is used to numerically advect the scalar. Various strategies for obtaining near-optimal protocols are compared with those obtained by random optimization methods.

Pattern Formation and Spatiotemporal Complex Dynamics in Extended Anisotropic Systems
Iuliana Oprea, Colorado State University, juliana@math.colostate.edu

This talk is particularly motivated by the spatiotemporal complex dynamics, especially the spatiotemporal chaos (STC), observed in the nematic electroconvection, a well-known example of a non-equilibrium driven anisotropic system. Since in anisotropic systems the minima on the neutral stability surfaces are isolated, they admit a unique reduced description through Ginzburg-Landau type amplitude equations. We present a comprehensive and systematic theoretical approach, through the study of Ginzburg Landau type amplitude and phase equations extracted from them, in the analysis of the specific mechanisms and features of the formation and dynamics of complex spatiotemporal patterns in the nematic electroconvection, and the formation of suncups. In the nematic electroconvection, as the patterns bifurcate at onset, theoretical results from normal form analysis are available in the characterization of the mechanisms generating them. Key questions we will address include what is the role of symmetry breaking of a chaotic attractor in the creation of STC, what are the routes to STC, what is the role of nonlinear interactions of wave patterns in the creation of spatiotemporal complex patterns, and which anisotropies are involved in their occurrence. This approach therefore allows for quantitative and qualitative comparison between the solutions of the model evolution equations and the experimental results, which should significantly increase the understanding of spatiotemporal complex patterns in anisotropic systems. This is a joint work with Gerhard Dangelmayr and Patrick Shipman at Colorado State University.

Estimating the Reproductive Number, Total Outbreak Size, and Reporting Rates for Zika Epidemics in Central & South America
Stephen Pankavich, Colorado School of Mines, pankavic@mines.edu

As an overwhelming number of nations within South and Central America are currently experiencing prolonged outbreaks of Zika virus, understanding important characteristics of these epidemics and how they vary across spatial regions is crucial to developing mitigation strategies to minimize ongoing and future infection. Utilizing data from the Pan American Health Organization (PAHO), we develop a new mathematical model for the 2015 Zika virus outbreak in Colombia, El Salvador, and Suriname and use tools from Approximate Bayesian Computation to estimate parameter distributions and provide uncertainty quantification. In addition to estimating the basic reproduction number within each affected nation, we further approximate nationwide reporting rates and the expected total size of each outbreak.

Physics, Innovation, and Entrepreneurship Explored Through Nonlinear Dynamics
Randall Tagg, University of Colorado at Denver

Nonlinear dynamics is a robust unifying framework for applying physics and mathematics to a wide range of real-world problems. We present a dozen “slices” of our Nonlinear PIE (Nonlinear Physics, Innovation, and Entrepreneurship) to demonstrate this versatility. Topics range from energy converters and actuators to waveguide optics to biomedical problems to fluid dynamics in materials processing. We use these projects to discover the types of learning that students need to consider career paths into innovation, industrial R&D, and entrepreneurship. This is part of the NSF “PIPELINE” grant to nine universities and the American Physical Society to create a wider community for helping students pursue careers through the application of physics and mathematics to innovation.

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MS09 "Methods of Applied and Numerical Complex Analysis"

Anna Zemlyanova, Kansas State University, azem@ksu.edu
Thomas DeLillo, Wichita State University, delillo@math.wichita.edu

An Introduction to Some Fourier Series Methods for Computing Conformal Maps to Exterior Simply and Multiply Connected Domains

Thomas DeLillo, Wichita State University, delillo@math.wichita.edu

We will give an overview of the numerical methods used in the following talk for approximating conformal maps from domains exterior to m circles to domains exterior to m given smooth curves. The methods use FFTs to compute Fourier and Laurent coefficients for the mapping functions. The methods are extensions of Fornberg's 1980 method for simply connected domains. Given the smooth target boundaries, the conformally equivalent circle domain must be found as part of the computation. A Newton-like method is used to compute the boundary correspondences and the centers and radii of the circles (the conformal moduli). The inner linear systems are discretizations of the identity plus a compact operator and can be solved efficiently with the conjugate gradient method.

An Electromagnetic Inverse Scattering Problem for Periodic Structures

Dinh-Liem Nguyen, Kansas State University, dlnguyen@ksu.edu

We consider the problem of shape reconstruction in inverse scattering of time-harmonic electromagnetic waves for periodic structures. We are interested in a class of periodic structures which are known as diffraction gratings. They are encountered in applications in optics such as diffractive optical filters and organic light-emitting diodes. The shape reconstruction problem under consideration, motivated by applications of non-destructive testing, can be formulated as an inverse problem. More precisely, given measurements of the scattered fields for a number of incident fields, we aim to reconstruct shape of the grating. We investigate the Factorization method introduced by A. Kirsch as an analytical as well as a numerical tool for solving this inverse problem. This method constructs a necessary and sufficient criterion whether a given point in space lies inside or outside the penetrable periodic structure, yielding a uniqueness result and a fast imaging algorithm. We provide a rigorous analysis for the method as well as numerical examples for visualizing efficiency of the method.

Computation of Plane Potential Flow Past Multi-element Airfoils Using Conformal Mapping, Revisited

Saman Sahraei, Wichita State University, sahraei@math.wichita.edu

We revisit methods for computing flow over single and multi-element airfoils using more recently developed numerical methods for conformal mapping for simply and multiply connected domains. The corners at the trailing edges of the airfoils are successively removed by Karman-Trefftz maps. The map from the domain exterior to disks to the domain exterior to the smooth images of the airfoils is computed using the Fourier series methods described in the preceding talk. The velocity potential for flow in the circle domain, with circulation calculated to satisfy the Kutta condition in the airfoil domain, is computed by a reflection method based on the Milne-Thompson Circle Theorem. Convergence of the reflection method is proven if the domains are sufficiently well-separated. This is joint work with T. DeLillo.

Surface Elasticity in Steigmann-Ogden Form in Modeling of Fracture

Anna Zemlyanova, Kansas State University, azem@ksu.edu

A problem of a straight mixed mode non-interface fracture in an infinite plane is treated analytically with the help of complex analysis techniques. The surfaces of the fracture are subjected to surface elasticity in the form proposed by Steigmann and Ogden. The boundary conditions on the banks of the fracture connect the stresses and the derivatives of the displacements. The mechanical problem is reduced to two systems of singular integro-differential equations which are further reduced to the systems of equations with logarithmic singularities. It is shown that modeling of the fracture with the Steigmann-Ogden elasticity produces the stress and strain fields which are bounded at the crack tips. The existence and uniqueness of the solution for almost all the values of the parameters is proved. Additionally, it is shown that introduction of the surface mechanics into the modeling of fracture leads to the size-dependent equations. A numerical scheme of the solution of the systems of singular integro-differential equations is suggested, and the numerical results are presented for different values of the mechanical and the geometric parameters.

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MS10 "Modeling, Computation, and Imaging of Pulmonary Activity"

Jennifer Mueller, Colorado State University, mueller@math.colostate.edu

D-bar Reconstructions with Prior Spatial Information for 2-D Human Thoracic EIT Data

Melody Alsaker, Gonzaga University, alsaker@gonzaga.edu

In this talk, we present the first-ever human data reconstructions computed using an a priori D-bar algorithm. Recent advances in direct D-bar reconstruction methods for Electrical Impedance Tomography have resulted in a priori techniques, in which prior information is included in the D-bar algorithm. If properly performed, these techniques lead to improved spatial resolution in the final reconstructions. One of the main challenges in these a priori methods has been the selection of estimates for conductivity values in the prior, since poor guesses can result in artifacts and distortions in the resulting reconstructions. This is especially evident in noisy human data sets. In this talk, we present an optimized and automated method for choosing conductivity values so as to mitigate artifacts and improve the reconstructions. We will present still frames and movies of human pulmonary data, showing tidal ventilation and PFT maneuvers, reconstructed using the new algorithm. We will also provide comparison images computed using a standard D-bar technique with no prior, to demonstrate the improved quality of the new reconstructions.

Results of a Study Deriving Pulmonary Function Measures from Functional Electrical Impedance Tomography in Children with Cystic Fibrosis

Michael Capps, Colorado State University, capps@math.colostate.edu

We will discuss the results of a study conducted on children with cystic fibrosis where we derive pulmonary function measures using functional electrical impedance tomography during a pulmonary function test, comparing the results with spirometry and a measure of heterogeneity derived from EIT data collected during tidal breathing.

Modeling as a Tool to Investigate Ventilator Induced Lung Injury

Michelle Mellenthin, University of Colorado Denver (Anschutz Medical Campus), michelle.mellenthin@ucdenver.edu

Damage to mechanically ventilated lungs is caused by overstretch and the repetitive collapse and reopening (recruitment and derecruitment, R/D) of alveoli. To assess the relationship between tissue damage with these mechanisms of injury, a numerical model that predicts distension and R/D was developed. The single compartment viscoelastic model was fit to lung mechanics measurements obtained from a study with mechanically ventilated mice. Half of the mice also received an injurious bronchoalveolar lavage (BAL). Dynamic pressure-volume (PV) loops were recorded every 5 min for the duration of the experiment. Predicted R/D and distension were determined for each PV loop using the numerical model and compared to BAL total protein concentration measured at the conclusion of the experiment. Our data suggests that rapid injury to the lung is more strongly associated with R/D and not overstretch.

Bayesian Framework for the Reconstruction of Anisotropic Conductivities in Electrical Impedance Tomography

Rashmi Murthy, Colorado State University, murthy@math.colostate.edu

Electrical Impedance Tomography (EIT) is a relatively new imaging technique that is non-invasive, low-cost, and non-ionizing with excellent temporal resolution. EIT data consists of electrical boundary measurements, of voltages measured on electrodes arising from applied currents on the electrodes, that are used to determine the unknown electrical conductivity in the interior of the medium. EIT has a variety of applications including medical imaging and geophysical prospecting. There have been quite a few advances in the study of EIT problem, particularly when the electrical conductivity is isotropic, that is direction independent. However, EIT with anisotropic conductivity, that is when the conductivity depends on direction of propagation, has not been studied in detail. Anisotropic EIT problem is of practical importance, since many tissues and organs in human body display anisotropy. Anisotropic EIT problem poses a mathematical challenge, in the sense that the problem does not have a unique solution. This talk presents a Bayesian approach to the anisotropic EIT problem to overcome the difficulty of non-unique solution to the problem.

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MS11 "Modeling the Immune Response to Infection"

Michael Kirby, Colorado State University, Michael.Kirby@ColoState.edu

Geometric Classification of Tolerant, Resistant and Susceptible Mice using Time Series Data

Manucher Aminian, Colorado State University

The broad goal of our research is to detect and characterize signatures related to the immune systems response to infection. In particular, we are interested in identifying features and patterns that capture the essence of distinct immune responses related to tolerance, resistance and susceptible reactions. To this end we explore the behavioral response of laboratory mice before and after being infected with Salmonella. The mouse body temperature and activity data are monitored at one sample per minute using surgically implanted telemetry devices. The resulting time series are analyzed using techniques from Machine Learning and dynamical systems analysis. This work is done in collaboration with Helene Andrews-Polymenis and David Threadgill of Texas A&M.

Centroid-Encoder Neural Networks for Data Visualization and Classification

Tomojit Ghosh, Colorado State University

For a given labelled data set one can expect to have a variance between the classes. At the same time we can also expect the intra-class variance is less than the inter-class variance. Although this assumption may not hold true for all data sets. But in practice this assumption might work in most of the cases. Keeping this assumption in mind we can say that the centroid is a good representative of the corresponding class. We hypothesized that a non-linear mapping from an input data to its corresponding centroid through low dimensional space might reveal some hidden structure in low dimensional space. A supervised learning algorithms is being proposed which exploit the class/category label information of each sample in a given labelled dataset. Based on Neural Network architecture this supervised algorithm maps each sample of class to the corresponding centroid of that class via a non-linear mapping. For visualization one can use a bottleneck layer with two/three hidden nodes to represent each sample in low dimensional space.

Sparse Support Vector Machines for Identifying Asympotomatic Shedders in the First 24 Hours

Ariel Liu, Colorado State University

Identifying asymptomatic shedders in the first 24 hours is a challenging and beneficial task in the field of infectious disease modeling and prediction. On one hand, it helps to prevent further infection and spread of the disease, on the other hand, it may lead to early diagnosis and treatment to the infected patients. Support Vector Machines are classifiers defined by a separating hyperplane where the samples are used to determine the hyperplanes parameters. Sparse support vector machines use a sparsity promoting L1-norm on the parameters which creates a powerful tool to identify not only asymptomatic shedders but also discriminative genes Currently with Sparse SVM the accuracy of our classification of gene expression data is over 80% in the first 24 hours.

A Dynamical Systems Approach to Real Time Anomaly Detection for Monitoring Infectious Disease

Xiaofeng Ma, Colorado State University

We propose a sequential algorithm for learning sparse radial basis approximations for streaming data and anomaly detection. The initial phase of the algorithm formulates the RBF training as a convex optimization problem with an L_1 objective function on the expansion weights while the data fitting problem imposed only as an L_∞-norm constraint. Each new data point observed is tested for feasibility, i.e., whether the data fitting constraint is satisfied. If so, that point is discarded and no model update is required. If it is infeasible, a new basic variable is added to the linear program. The result is a primal infeasible-dual feasible solution. The dual simplex algorithm is applied to determine a new optimal solution. The data point causes infeasibility can be considered as novel data point, which indicates where anomaly rises. A large fraction of the streaming data points does not require updates to the RBF model since they are similar enough to previously observed data and satisfy the data fitting constraints. The structure of the simplex algorithm makes the update to the solution particularly efficient given the inverse of the new basis matrix is easily computed from the old inverse. We illustrate the method on time-series of temperature data collected from mice. In this case we can see this anomaly detection model identifies the points when there was exposure to the pathogen and subsequent changes in behavior.

Generative Adversarial Neural Networks for Learning Contagion

Lange Simmons, Colorado State University

A common problem with machine learning on biological datasets is the lack of data and the expense of creating new data. There are many ways around this problem, but one of them could be the use of networks that learn the distribution of the existing data's classes to produce "counterfeit" data to augment the training of the ML model. Generative adversarial networks use two neural networks, one that creates data matching a given label, and another that aims to distinguish between the fabricated data and the data from the training set comprised of actual data as proposed by Goodfellow. This leads to a network that can produce many samples of the desired class. In the case of contagion gene expression data, this can allow unbalanced classes to be balanced much like an algorithm such as SMOTE would do. We illustrate how this approach can be used to augment the available data and present a machine learning application.

Manifold Learning Techniques for Visualizing Temporal Biomarkers

Shannon Stiverson, Colorado State University

Early diagnosis of respiratory viral infections (RSVs) is essential for facilitating treatment as well as preventing spread of the disease. In light of this, we wish to identify biomarkers of RSVs in humans and visualize temporal changes in the signals from these biomarkers. Manifold learning techniques are applied to differential gene expression data from subjects inoculated with various RSVs to visualize changes throughout the course of infection. We explore a technique known as Sparse Manifold Clustering and Embedding for uncovering the underlying structure of the data and visualize temporal trajectories. Results are compared with those from the related algorithm for locally linear embedding (LLE). In addition, a new approach applying LLE on Grassmann manifolds is discussed.

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MS12 "Models and Methods for Problems in Applied Mathematics"

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Biomechanics of Micro-Colony Morphology in Cyanobacteria
Sabina Altus, University of Colorado at Boulder, sabina.altus@colorado.edu

Photosynthesis is regulated by individual cells in response to their environment; however, improving efficiency at the larger, micro-colony scale requires a full biomechanical picture of cell-to-colony dynamics. Colonies grown under a substrate, and with no boundary constraint, are observed to spatially self-organize into round colonies with regions of cells all oriented in the same direction (similar to the nematic regions seen in liquid crystals). In this work, a biomechanical model is presented to simulate micro-colony morphology, including formation of these regions, principally guided by competing forces from cell-cell interaction, cell growth and interaction with the substrate. Results from this ongoing work will be presented.

A Variable Nonlinear Splitting Algorithm for Reaction Diffusion Systems with Self and Cross-diffusion
Matthew A. Beauregard, Stephen F. Austin State University, beauregama@sfasu.edu

Self and cross-diffusion are important nonlinear spatial derivative terms that are included into biological models of predator-prey interactions. Self-diffusion models overcrowding effects, while cross-diffusion incorporates the response of one species in light of the concentration of another. In this talk, a new nonlinear operator splitting method is presented that directly incorporates both self and cross-diffusion into a computational efficient design. The numerical analysis guarantees the accuracy and criteria for stability. Numerical experiments display its efficiency in simulating a generalized Shigesada-Kawasaki-Teramoto (SKT) model. This is a joint work with Joshua Padgett at Texas Tech University and Rana Parshad at Clarkson University.

Modeling of Chirped Gratings Based on Interferometric Lithography
Steve Benoit, Colorado State University, benoit@math.colostate.edu

Interferometric lithography with curved wavefronts produces chirped gratings. The chirp can be longitudinal with the periodicity changing along the grating wavevector or transverse with the periodicity changing in the perpendicular direction. The chirp is investigated for a range of configurations and specific optical systems to generate a wide range of grating chirp parameters that are analyzed.

Modified Radon Transform Inversion Using Moments
Regene DePiero, University of Wyoming, rdepiero@uwyo.edu

A modified Radon transform via convolution with a mollifier is established and its inversion formula is obtained. The problem of recovering the bivariate function from the moments of its Radon transform data is considered. We show how the moments of the Radon transform can be extracted from the moments of the modified Radon transform and use this relationship to provide a uniform approximation to the original function.

Sensitivity and Bifurcation Analysis for a Differential-Algebraic Equation Model of a Microbial Electrolysis Cell
Harry Dudley, University of Colorado Boulder, Harry.Dudley@Colorado.edu

Microbial electrolysis cells (MECs) are a promising new technology for producing hydrogen cheaply, efficiently, and sustainably. The technology is based on microbial fuel cells in which bacteria oxidize a substrate to generate current, decreasing electricity costs. MECs are more efficient than fermentation methods and can be fed fermentation effluent or cheap and readily available wastewater. However, to scale up this technology, we need a better understanding of the processes in the devices. In this effort, we present a sensitivity analysis for a differential-algebraic equation (DAE) model of a batch-fed microbial electrolysis cell with an algebraic constraint on current. We conduct both differential sensitivity analysis and principle component analysis after fitting simulations to current density data. The former suggests which parameters have the greatest influence on the current density at particular times during the experiment. The latter reveals relationships between sets of unknown parameters, including microorganism growth and consumption rates and half rate constants. We also plan a numerical bifurcation study to identify the stability of equilibrium points as well as possible bifurcations.

A Dimension Reduction Method for Time-Series Prediction
Mahsa Ghorbani, Colorado State University, mahsa.ghorbani@colostate.edu

In this talk we focus on a time-series prediction method for stock prices. The literature provides strong evidence that prices can be predicted from past price data as well as other fundamental and macroeconomic variables. Principal component analysis (PCA) is a widely used mathematical technique for dimensionality reduction and analysis of data by identifying a small number of principal components to explain the variation found in a data set. In this paper, we described a general method for stock price prediction using covariance information based on principle components. We illustrate our method on daily stock price values for General Electric Company. The daily historical price data from 1996 to 2015 are transformed into matrices of different lengths to investigate the impact of length of observation on estimation power. We investigate the results based on mean square error of prediction, as a measure of performance, and volatility of prediction as a measure of risk.

A Demonstration of the Julia Programming Language
Derek Handwerk, Colorado State University, handwerk@math.colostate.edu

Julia is a high-level, high-performance dynamic programming language for technical computing. It was designed from the ground up to be easy to program like Python or MATLAB, yet have speeds approaching C and Fortran. An overview of the language will be given as well as interactive examples.

Matrix Spectral Factorization
Fritz Keinert, Iowa State University, keinert@iastate.edu

A causal finite impulse response filter bank is described by thematrix polynomial\begin{equation*} H(z) = \sum_{k=0}^n H_k z^{-k},\end{equation*}where the coefficients H_k are $r \times r$ matrices. Its adjoint is\begin{equation*} H^*(z) = \sum_{k=0}^n H_k^* z^k,\end{equation*}and the product filter is given by\begin{equation*} P(z) = H(z) H^*(z).\end{equation*}Obviously, $P(z)$ is positive semidefinite for every $z \in {\mathbb C}$, $z \ne 0$.The problem of {\em matrix spectral factorization} is to recover$H(z)$, given a positive semidefinite $P(z)$. We are interested inthis in the context of multiwavelet design.It is known that this factorization is possible. Many algorithms havebeen proposed, but most of them fail if $P(z)$ is not strictlypositive definite on the unit circle (the {\em degenerate case}). Inaddition, the solution in the degenerate case can only be found withreduced accuracy, and convergence is very slow. However, this isexactly the case we are interested in.I will discuss a particular algorithm by Youla and Kazanjian, whichcan handle the degenerate case, and various attempts to speed up itsconvergence, and improve accuracy.

Interactions of Solitary Waves and Compression/Expansion Waves in Core-annular Flows
Michelle Maiden, University of Colorado at Boulder, Michelle.Maiden@Colorado.edu

The nonlinear hydrodynamics of an initial step leads to the formation of rarefaction waves and dispersive shock waves in dispersive media. Another hallmark of these media is the soliton, a localized traveling wave whose speed is amplitude dependent. Although compression/expansion waves and solitons have been well-studied individually, there has been no mathematical description of their interaction. In this talk, the interaction of solitons and shock/rarefaction waves for interfacial waves in viscous, miscible core-annular flows are modeled mathematically and explored experimentally. If the interior fluid is continuously injected, a deformable conduit forms whose interfacial dynamics are well-described by a scalar, dispersive nonlinear partial differential equation. The main focus is on interactions of solitons with dispersive shock waves and rarefaction waves. Theory predicts that a soliton can either be transmitted through or trapped by the extended hydrodynamic state. The notion of reciprocity is introduced whereby a soliton interacts with a shock wave in a reciprocal or dual fashion as with the rarefaction. Soliton reciprocity, trapping, and transmission are observed experimentally and are found to agree with the modulation theory and numerical simulations.

A Numerical Method for the Quantum Liouville-BGK Equation
Sophia Potoczak, Colorado State University, potoczak@math.colostate.edu

This talk will introduce a numerical scheme for solving the quantum Liouville-BGK equation, where the equilibrium in the relaxation term is obtained by minimizing a free energy functional under local constraints. The equation forms a system of coupled nonlinear PDEs and models the dynamics of a many-particle system. The numerical difficulties lie in the nonlinear coupling between the PDES, and are addressed by using a splitting scheme in which the nonlinearity becomes a perfectly linear term. We will discuss the specifics of the scheme and present related numerical results.

On Stochastic Boussinesq Equations
Geordie Richards, Utah State University

We will review some recent results on stochastic Boussinesq equations, which are model equations for Rayleigh-B\'{e}nard convection perturbed by an additive noise. First we will discuss ergodicity and mixing results in the two-dimensional periodic domain with white noise activated on a few low Fourier modes. These results generalize contributions of Hairer and Mattingly on hypo-ellipticity for semilinear stochastic PDEs. Then, with a rougher forcing but more physical boundary conditions, we present a simplified proof of ergodicity, and discuss the convergence of observables, such as the Nusselt number, in the infinite Prandtl number limit. Finally, we will report on a stochastic approach to hydrodynamic stability, and on the influence of fast rotation terms.

Modeling Light Propagation in Tissues
Shelley Rohde, Metropolitan State University of Denver, srohde2@msudenver.edu

This talk will outline a diffuse optical tomography problem applying a corrected diffusion approximation to determine optical properties of tissues. Specifically, a model using an obliquely incident Gaussian beam on a layered medium. The results of this model use reflectance measurements to determine epithelial tissue properties. This talk will also address an extension to diffuse optical spectroscopy using a pulsed beam from a recent paper.

Discrete Miranda-Talenti Estimates and Applications to Linear and Nonlinear PDEs
Mohan Wu, University of Pittsburgh, mow11@pitt.edu

In this talk, we construct simple and convergent fnite element methods for linear and nonlinear elliptic differential equations in non-divergence form with discontinuous coefficients The methods are motivated by discrete Miranda-Talenti estimates, which relate the H2 semi-norm of piecewise polynomials with the L2 norm of its Laplacian on convex domains. We develop a stability and convergence theory of the proposed methods, and back up the theory with numerical experiments.

Lowest-order Weak Galerkin Finite Element Method for Darcy Equation on Polygonal Meshes
Zhuoran Wang, Colorado State University, zhrwang@rams.colostate.edu

In this talk, we present the lowest-order weak Galerkin (WG) finite element method for solving the Darcy equation on general convex polygonal meshes. In this approach, we approximate the pressure by constants inside elements and on edges. The discrete weak gradients of these constant basis functions are defined in an H(div)-subspace that is constructed by using the normalized coordinates and Wachspress coordinates. This new WG method is locally mass-conservative, and produces continuous normal fluxes. Numerical results are presented to demonstrate its 1st order accuracy in pressure, velocity, and flux.

Perspectives on Exponential Random Graphs
Mei Yin, University of Denver, mei.yin@du.edu

Large networks have become increasingly popular over the last decades, and their modeling and investigation have led to interesting and new ways to apply analytical and statistical methods. The introduction of exponential random graphs has aided in this pursuit, as they are able to capture a wide variety of common network tendencies by representing a complex global structure through a set of tractable local features. This talk will offer various perspectives on large exponential random graphs. The main techniques that we use are variants of statistical physics but the exciting new theory of graph limits, which has rich ties to many parts of mathematics and beyond, also plays an important role in the interdisciplinary inquiry. Based on joint work with multiple collaborators.

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MS13 "Novel Numerical Methods for Multiphysics Problems"

Lin Mu, Oak Ridge National Lab, jraver@gmail.com
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Xiu Ye, University of Arkansas at Little Rock, xxye@ualr.edu

Numerical Modeling of Incommensurate 2D Moir Atomic Structures via C* Algebras

Paul Cazeaux, University of Kansas, pcazeaux@ku.edu

Weak van der Waals interactions between 2D materials layers do not impose limitations on integrating highly disparate materials such as graphene, hexagonal boron nitride and many others. This is both a blessing, allowing the realization of many more configurations, and a curse from a modeling perspective due to the loss of periodicity. Unusual geometries appear at the atomic-scale, such as lattice mismatches, twist angles and Moire patterns, providing new challenges for our fundamental understanding. Dynamic and macroscopic properties of such aperiodic condensed matter systems can be formulated in the framework of C*-algebras introduced by Bellissard and his co-authors. I will present our recent efforts towards an effective computational implementation of these abstract objects.

Superconvergence of PN Equations on Linear Kinetic Equations

Zheng Chen, Oak Ridge National Laboratory, chenz1@ornl.gov

We prove some convergence properties for a semi-discrete, moment-based approximation of a model kinetic equation in one dimension. This approximation is equivalent to a standard spectral method in the velocity variable of the kinetic distribution and, as such, is accompanied by standard algebraic estimates of the form N^{-q}, where N is the number of modes and q depends on the regularity of the solution. However, in the multiscale setting, we show that the error estimate can be expressed in terms of the scaling parameter ϵ, which measures the ratio of the mean-free-path to the characteristic domain length. In particular we show that the error in the spectral approximation is $\mathcal{O}(\epsilon^{N+1})$. More surprisingly, the coefficients of the expansion satisfy some super convergence properties. In particular, the error of the ℓ^{th} coefficient of the expansion scales like $\mathcal{O}(\epsilon^{2N})$ when $\ell =0$ and $\mathcal{O}(\epsilon^{2N+2-\ell})$ for all $1\leq \ell \leq N$. This result is significant, because the low-order coefficients correspond to physically relevant quantities of the underlying system. All the above estimates involve constants depending on N, time t and initial condition. We also investigate how these constants change along N, since we would like to have an extra power in ϵ while using larger P_N system. Numerical tests will also be presented to support the theoretical results.

Wavelet Method for Eigenvalue Problem

Ruihao Huang, Michigan Technological University, ruihaoh@mtu.edu

The elliptic eigenvalue problems have been widely used in many applications including vibration modes simulation in acoustics, nuclear magnetic resonance approximation and etc. In this project, we will solve the elliptic eigenvalue problem based on wavelet method. Historically, wavelet methods were designed to solve PDE source problem, with arbitrary s order only related to wavelet itself. Our current work is based on sparse grid and it can reduce the computational cost significantly, which keep almost the same accuracy. The future work will focus on adaptive wavelet method for eigenvalue computation.

A Trefftz Discontinuous Galerkin Method for Time-Harmonic Waves with a Generalized Impedance Boundary Condition

Shelvean Kapita, University of Georgia, shelvean.kapita@uga.edu

We show how a Trefftz Discontinuous Galerkin (TDG) method for the displacement form of the Helmholtz equation can be used to approximate problems having a generalized impedance boundary condition (GIBC) involving surface derivatives of the solution. Such boundary conditions arise naturally when modeling scattering from a scatterer with a thin coating. The thin coating can then be approximated by a GIBC. A second place GIBCs arise is as higher order absorbing boundary conditions. This paper also covers both cases. Because the TDG scheme has discontinuous elements, we propose to couple it to a surface discretization of the GIBC using continuous finite elements. We prove convergence of the resulting scheme and demonstrate it with two numerical examples.

A Modified Weak Galerkin Finite Element Method

Nolisa Malluwawadu, University of Arkansas at Little Rock, nsmalluwawad@ualr.edu

The modified weak Galerkin method is a combination of processes used in the weak Galerkin (WG) and the discontinuous Galerkin (DG) methods for the second order Poisson equation. First, we define a new discrete weak gradient operator. This enables us to draw strengths from both WG and DG methods. Ease of implementation and flexibility from WG and same benefits as DG but with easier implementation. This method also enables us to have a single stabilizer without having to worry about the parameter being sufficiently large. The method have the optimal order convergence rates.

Error Estimate for New Weak Galerkin Finite Element Methods

Lin Mu, Oak Ridge National Laboratory, mul1@ornl.gov

In this talk, we will introduce the new developed weak Galerkin finite element methods, which is making use of weak functions. The new weak Galerkin approach is positive definite, symmetric, and can be applied on the polygonal shape of elements. The optimal rate in convergence will be shown theoretically and numerically.

Stabilized Discretizations for Poroelasticity and Stokes' Equations

Peter Ohm, Tufts University, peter.ohm@tufts.edu

In this talk, the popular P1-RT0-P0 discretization of the three-field formulation of Biot's consolidation problem will be discussed. In general, this finite element formulation does not satisfy an inf-sup condition uniformly with respect to the physical parameters and, thus, several issues arise in when using it in numerical simulations. Here, we propose a stabilization technique that enriches the piecewise linear finite-element space of the displacement field with the span of edge/face bubble functions. For Biot's model, this gives rise to discretizations that are uniformly stable with respect to the physical parameters. Additionally, a perturbation of the bilinear form is done, which allows for local elimination of the bubble functions, providing a uniformly stable scheme with the same number of degrees of freedom as the classical P1-RT0-P0 approach. Finally, this scheme is also successfully applied to Stokes equations, yielding a discrete problem with optimal approximation properties and with a minimum number of degrees of freedom (equivalent to a P1-P0 discretization). Numerical tests confirm the theory for both poroelastic and Stokes test problems.

A Posteriori Error Analysis on Polytopal Meshes and Simple Methods for the Problems with Non-divergence Forms

Xiu Ye, University of Arkansas at Little Rock, xxye@ualr.edu

The goal of this talk is twofold. First, a posteriori error estimators have been developed for both the weak Galerkin and the discontinuous Galerkin finite element methods. The most existing a posteriori error analysis only work on simplicial elements even for the polygonal and polyhedral finite element methods. Our new residual type estimators can be applied to general meshes such as hybrid mesh, polytopal mesh and mesh with hanging node. In addition, these estimators consist fewer terms and are easy to compute. Second, we present simple finite element methods for solving some non-classical problems such as second order elliptic equations in non-divergence form, Cauchy problem and simple hyperbolic problem. Error analysis have been provided and extensive numerical examples have been tested.

An Immersed Discontinuous Finite Element Method for the Stokes Problem with a Moving Interface

Pengtao Yue, Virginia Tech, ptyue@math.vt.edu

We present a discontinuous immersed finite element (IFE) method for incompressible interfacial flows that are governed by the Stokes equations. The method is based on a Cartesian mesh with elements cut by the moving interface. On this fixed unfitted mesh, we employ an immersed Q_1/Q_0 finite element space constructed according to the location of the interface and pertinent interface jump conditions. As such, the smearing of solution across the interface is greatly reduced. The interface, represented by a sequence of marker points, is advected on the fixed background mesh by the local fluid velocity. The mesh is locally refined near the interface to further improve accuracy. Compared with the phase-field method on adaptive meshes, our method can achieve the same level of accuracy with much less degrees of freedoms. We present some numerical examples to validate and demonstrate the capability of the proposed method.

Superconvergence of Immersed Finite Element Methods and Finite Volume Methods

Xu Zhang, Mississippi State University, xuzhang@math.msstate.edu

Immersed finite element method (FEM) and finite volume method (FVM) are numerical methods for solving interface problems with unfitted meshes. Superconvergence is a phenomenon that the order of convergence at certain points is higher than the maximum order of convergence of numerical solutions. In this talk, we present some superconvergence properties of Immersed FEM and immersed FVM for one dimensional interface problems. The key step in our analysis is the construction of generalized orthogonal polynomials with discontinuous weight function. We will show that the immersed FEM and FVM will inherit all desired superconvegence properties from standard FEM. Some numerical examples will be presented.

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MS14 "Efficient Methods for PDEs and Applications"

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Lowest-order Weak Galerkin Finite Element Methods for Elasticity on Quadrilateral and Hexahedral Meshes

Graham Harper, Colorado State University, harper@math.colostate.edu

This talk presents the lowest-order weak Galerkin finite element methods for linear elasticity on quadrilateral and hexahedral meshes. Methods for optimizing the numerical implementation are discussed, and numerical experiments on several examples are presented to illustrate properties including first order convergence in stress, first order convergence in displacement, and the desirable locking-free property.

A Weak Galerkin Finite Element Method for Second Order Elliptic Problems with Mixed Boundary Conditions

Saqib Hussain, University of Arkansas at Little Rock, sxhussain@ualr.edu

In this talk, a weak Galerkin finite element method is proposed and analyzed for the second order elliptic equation with mixed boundary conditions. Wang and Ye were the first two authors to introduce and analyze the weak Galerkin method for the second order elliptic problems. The basic idea of the weak Galerkin method is to use the weak functions and their weak derivatives in the approximation. The talk will start with the second order elliptic equation with the mixed boundary condition, for which weak Galerkin finite element methods shall be applied and explained in detail. Error estimates of the optimal order will be established for the corresponding weak Galerkin approximations in both a discrete H1 norm and standard L2 norm. In the end, we will present numerical experiments to verify the efficiency of the method.

Efficient Time Domain Decomposition Algorithms for PDE-constrained Optimization Problems

Jun Liu, Southern Illinois University Edwardsville, juliu@siue.edu

Optimization with time-dependent partial differential equations (PDEs) as constraints appear in many engineering applications. The associated first-order necessary optimality system consists of one forward and one backward time-dependent PDE coupled with optimality conditions. An optimization process by using the one-shot method determines the optimal control, state, and adjoint state at once at the cost of solving a large scale, fully discrete optimality system. Hence, such one-shot methods could easily become prohibitive when the time span is long or a small time step is taken. To overcome this difficulty, we propose in this paper several time domain decomposition algorithms for improving the computational efficiency. In these algorithms, the optimality system is split into many small subsystems over a much smaller time interval, which are coupled by appropriate continuity matching conditions. Both one-level and two-level multiplicative and additive Schwarz algorithms are developed for iteratively solving the decomposed subsystems in parallel. In particular, the convergence of the one-level multiplicative and additive Schwarz algorithms without overlap are proved. The effectiveness of our proposed algorithms is demonstrated by both 1D and 2D numerical experiments, where the developed two-level algorithms show very scalable convergence rates with respect to the number of subdomains.

A Multi-scale Model for Optical Responses of Nano-structures

Songting Luo, Iowa State University, luos@iastate.edu

We present a semi-classical model for studying the optical responses of nano-structures, where the wave propagation is determined classically through Maxwell's equations and the motion of the nano-structure is determined quantum mechanically through Schrodinger's equation. Ehrenfest molecular dynamics and Density Functional Theories are applied to deal with the many-body Schrodinger equation. The semi-classical model is numerically traceable. Linear response formulations will be derived and multi-scale solvers will be designed to solve the model. Numerical examples will be presented to demonstrate the model. This is a joint work with Gang Bao and Di Liu.

Validating a Dynamic Wildfire Risk PDE Model
Alex Masarie, Colorado State University, alex.masarie@gmail.com

Cooperative wildfire management in the United States represents an advanced human cognitive task. Careful allocation of fire personnel to small, routine fire incidents as well as large, dangerous ones is necessary for safe, effective response. We explore the dynamics of sharing specialized ground-based suppression resources across regional management boundaries focusing on the heat of summer when there is little margin for miss-appropriating a crew. We build a model for continuous demand potential and thus trade potentially complicated heuristic modeling for a heat-type partial differential equation (PDE) identification. Still a complicated problem, we reduce to a tractable basis of regional risk metrics like ongoing activity, suppression resource use, weather, expenditures, accessibility, and population density. This talk will describe smoothing methods for these discrete data representors on structured meshes that conformed to regional management boundaries. By inverting finite difference matrices we leverage Crank-Nicholson convergence to fit daily risk factor models. We characterize the spatiotemporal stochasticity in best-fit risk coefficients by calculating their spectra and semi-variograms. Visualizing our results indicates the various cognitive interpretations of correlated risks manifest as chaotic dynamics. But, the application of these PDE methods afford a deeper look into driving factors and risk gradient alignment.

A Two-sided Fractional Conservation of Mass Equation
Aleksey Telyakovskiy, University of Nevada, Reno, alekseyt@unr.edu

A two-sided fractional conservation of mass equation is derived by using left and right fractional Mean Value Theorems. This equation extends the one-sided fractional conservation of mass equation of Wheatcraft and Meerschaert. We show how to derive a two-sided fractional advection-dispersion equation. The derivations are based on Caputo fractional derivatives. This is a joint work with Jeffrey Olsen and Jeff Mortensen.

A Space-time Fractional Phase-field Model with Tunable Sharpness and Decay Behavior
Hong Wang, University of South Carolina, hwang@math.sc.edu

We present a space-time fractional Allen-Cahn phase-field model that describes the transport of the fluid mixture of two immiscible fluid phases. The space and time fractional order parameters control the sharpness and the decay behavior of the interface via a seamless transition of the parameters. Although they are shown to provide more accurate description of anomalous diffusion processes and sharper interfaces than traditional integer-order phase-field models do, fractional models yield numerical methods with dense stiffness matrices. Consequently, the resulting numerical schemes have significantly increased computational work and memory requirement. We develop a lossless fast numerical method for the accurate and efficient numerical simulation of the space-time fractional phase-field model. Numerical experiments shows the utility of the fractional phase-field model and the corresponding fast numerical method.

Maximum Principles for P1-P0 Weak Galerkin Finite Element Approximations of Quasi-linear Second Order Elliptic Equations
Ran Zhang, Jilin University, zhangran@jlu.edu.cn

This talk will introduce maximum principles for the weak Galerkin method dealing with the second order elliptic equation. Under the h-acute assumption for the mesh partition, two maximum principles with respect to midpoints are proved. The theoretical analysis is based on the variational form and De Giorgi technique. Some numerical results are also presented.

Adaptive C^0 Interior Penalty Methods for a Fourth Order Variational Inequality
Yi Zhang, University of North Carolina at Greensboro, y_zhang7@uncg.edu

We consider the displacement obstacle problem of clamped Kirchhoff plates which is formulated as a fourth order variational inequality, and we develop an a posteriori analysis of C^0 interior penalty methods. We discuss reliability and efficiency estimates for the residual based error estimator and introduce an adaptive algorithm. We will present numerical results to gauge the performance of the adaptive quadratic and cubic C^0 interior penalty methods. This is joint work with Susanne Brenner, Joscha Gedicke, and Li-yeng Sung.

Numerical Approximations for a Three-component Cahn-Hilliard Phase-field Model
Jia Zhao, Utah State University, jia.zhao@usu.edu

How to develop efficient numerical schemes while preserving energy stability at the discrete level is challenging for the three-component Cahn-Hilliard phase-field model. In this talk, we develop a set of first and second order temporal approximation schemes based on a novel energy quadratization (EQ) approach, where all nonlinear terms are treated semi-explicitly. Consequently, the resulting numerical schemes lead to well-posed linear systems with symmetric, positive definite operators to be solved at each time step. We rigorously prove that the developed schemes are unconditionally energy stable and present various 2D and 3D numerical simulations to demonstrate the stability and the accuracy of the schemes. This is a joint work with Xiaofeng Yang (University of South Carolina), Qi Wang (University of South Carolina), and Jie Shen (Purdue University).

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MS15 "Interactions among Analysis, Optimization and Network Science"

Pietro Poggi-Corradini, Kansas State University, pietro@math.ksu.edu
Nathan Albin, Kansas State University, albin@math.ksu.edu

A Modulus Framework in Broad Strokes

Nathan Albin, Kansas State University, albin@math.ksu.edu

Modulus on discrete networks is a natural analog of modulus of curve families in metric space and, as such, provides a flexible framework for describing the structures of graphs. Starting from the basic definitions, this talk will provide a broad summary of the theory and applications of modulus our group has been developing over several years. Theoretical topics include the abstraction of modulus to families of "objects", the application of Fulkerson's blocking duality to establish a strong connection between each family of objects and a particular dual family, and the probabilistic interpretation of modulus and its relationship to minimum expected overlap problems. Applications of modulus are various, depending on the particular family of objects selected. This talk will describe several such applications including "modulus metrics" (generalizing well-known metrics based on minimum cut, effective resistance, and shortest path), centrality measures (based on "shell modulus"), community detection (based on "loop modulus"), and an interesting hierarchical graph decomposition (based on spanning tree modulus).

Leveraging Multiple Networks for Enhanced Recommendations

Doina Caragea, Kansas State University, dcaragea@ksu.edu

Recommender systems provide users with personalized item recommendations by identifying patterns in past user-item preference networks. Traditional approaches to recommender systems work on a single network, i.e., use preferences for items of one type (e.g., books) and recommend items of the same type. However, users generally interact with items of multiple types (e.g., books, places, friends). Current Web technologies enable the collection, storage, and linking of multiple related user-item preference networks. Consequently, cross-network recommender systems that use additional source networks to enhance the recommendations for a target network have emerged recently. We present two neighborhood-based approaches that aggregate knowledge from multiple user-item preference networks, under the assumption that there is overlap between users in different networks, but the items are of different types (e.g., the items recommended to a researcher can be collaborators, papers to read and conferences to attend). Our approaches rely on the Adsorption algorithm, which makes recommendations to a user by propagating information from the neighbors of that user. Experimental results on datasets collected from DBLP and Last.FM show that our cross-network approaches can improve the recommendation accuracy in the target network as compared to approaches that use only the target network.

Modulus Metrics on Networks

Thiwanka Fernando, Kansas State University, tnethali@ksu.edu

Three classical network metrics are shortest path, effective resistance and the (reciprocal of) minimum cut. Modulus is a way to quantify the richness of families of objects on graphs, such as families of walks, trees, cycles etc...Here we focus on families of walks. First we recall its definition. For 1 ? p < ?, the p-modulus of a family ? is Mod_p(?) := inf ? ?(e)^p (the sum over e?E and inf over ??Adm(?)), where ? : E ? [0,?) is admissible for ? (? ? Adm(?)) if l_?(?) := ? N(?,e)?(e) ? 1 ?? ? ? (the sum over e?E), here N(?,e) is the number of times ? crosses the edge e. Let ?(a,b) be the connecting family of all walks from a to b. Fix 1 < p < ? and let q := p/(p?1) be the Holder conjugate exponent. Then, our main result shows that,?_p(a,b) := Mod_p(?(a,b))^{?q/p} is a metric on V .Our proof relies on Fulkerson Duality for p-modulus and, since ?_2 is effective resistance, in the case p = 2 this gives a new proof that effective resistance is a metric. Also as p??, ?_p is shortest path; and for 1 < p < 2, Mod_p(?(a,b))^{?1} is a metric and it tends to the reciprocal of mincut as p ? 1, thus recovering all three classical metrics. Finally, the result is sharp, in the sense that for every ? > 0, ?_p^{1+?} is not a graph metric in general.

Conformal Dimension and Graph Approximations
Lukas Geyer, Montana State University, geyer@montana.edu

Combinatorial p-modulus on a family of graph approximations has been successfully used to find numerical approximations to the conformal dimension of the Sierpinski carpet. We present generalizations of this method to other self-similar sets such as Julia sets of rational maps and limit sets of Kleinian groups.

A Practical Anytime Algorithm for Bipartite Networks
Timothy Goodrich, North Carolina State University, tdgoodri@ncsu.edu

Bipartite networks are naturally occurring optimization problems in domains where bipartite structure has specific meaning, such as in computational biology and quantum computing. We develop a new anytime algorithm for bipartite networks using a refined iterative compression routine proposed in the parameterized complexity literature. We improve the practical performance of this routine by introducing gray codes and a maximum flow solver for dynamic graphs. In addition, we prune the input network using reduction routines and linear-time approximation algorithms, resulting in fast and reasonable initial solutions. In contrast to existing state-of-the-art bipartite network solvers such as IBM's CPLEX linear programming solver and Iwata and Akiba's vertex cover solver, our method naturally lends itself to parallel computing. As a proof of concept, we apply our method to quantum annealer compilation, where compilers use bipartite networks to embed program graphs into a bipartite hardware fabric.

Gradient Young Measures and Functions of Exponentially Integrable Distortion
Christopher Halverson, Saint Louis University, halverson@slu.edu

We aim to extend the result of Astala and Faraco, and show, under certain constraints, if a sequence of Gradient Young Measures is K(z) quasi-regular, then it can be generated by a sequence of functions with exponentially integrable distortion.

Using Loop Structure to Detect Communities in Networks
Michael Higgins, Kansas State University, mikehiggins83@gmail.com

Community detection in networks is an important problem in Statistics, Computer Science, and the Social Sciences. Communities are defined by the presence of edges: edges are more abundant between vertices within the same community than across different communities. Hence, loops may be more prevalent within a community, and identifying locations where loops are abundant may be helpful in detecting communities. In this talk, we discuss current popular methods for discovering communities. We then describe how measures of loop prevalence--for example, loop modulus and the location of terminal edges in non-reversible random walks--can be used to enhance these methods.

Hardy-Sobolev Inequalities in Metric Measure Spaces
Lizaveta Ihnatsyeva, Kansas State University, ihnatsyeva@ksu.edu

In the talk I would first like to consider Muckenhoupt A_p properties of the powers of distance functions. Then I will discuss Hardy-Sobolev inequalities with such sort of distance weights. These inequalities form a natural interpolating scale between the (weighted) Sobolev inequalities and the (weighted) Hardy inequalities. The talk is based on a joint work with B. Dyda, J. Lehrbäck, H. Tuominen and A. Vähäkangas.

Random Trees via Conformal Welding
Peter Lin, University of Washington, peterlin@uw.edu

Every finite combinatorial tree can be canonically embedded in the plane as the solution to a certain conformal welding problem. We consider the properties of this embedding for large random trees. In particular we investigate the existence, uniqueness and regularity of the limiting probability distribution as the number of edges goes to infinity. This is based on joint work with Steffen Rohde.

Hierarchical Cluster Analysis via Network Flow Duality

David Matula, Southern Methodist University, matula@smu.edu

We present a clustering method based on the fundamental graph-theoretic concept of density (i.e., sparse cuts separating dense clusters) and implemented via a duality to peer-to- peer network flow between all pairs. The maximum concurrent flow problem (MCFP) can be formulated as an LP with maximin objective to maximize the flow throughput guaranteed between all node pairs subject to the path flow's sharing capacity of the edges. Throughput is the ratio of the flow delivered between a node pair in comparison to the node pair's corresponding demand. Employing LP duality, the optimal throughput is shown to determine a critically saturated separating set of edges partitioning the network into component parts, where all edges of the components have strictly positive residual capacity. The hierarchical MCFP (HMCFP) then further maximizes throughput in the residual capacity components determining a second throughput level and set of critical edges; iterating further, a series of throughput levels is determined until all edges are critical, yielding a stratification portrayed in clustering and classification theory as a dendrogram. The duality between sparsest cuts and MCF provides a natural characterization and foundation for the often stated, somewhat vague expression that objects in the same cluster (component) have more affinity (connectivity) to each other, and objects in different clusters are relatively less similar (sparsely connected).

Stolarsky Principle and Energy Optimization on the Sphere

Ryan Matzke, University of Minnesota, matzk053@umn.edu

The classical Stolarsky invariance principle connects the spherical cap L^2 discrepancy of a finite point set on the sphere to the pairwise sum of Euclidean distances between the points. We can extend this notion to use different notions of discrepancy to use on problems of discrete energy optimization. In particular, we can find the maximum value of the pairwise sum of geodesic distances of points on the sphere, as well as what arrangements produce that maximum.

Dirichlet Graph Partitions

Braxton Osting, University of Utah, osting@math.utah.edu

I'll discuss a geometric approach to graph partitioning where the optimality criterion is given by the sum of the first Dirichlet-Laplacian eigenvalues of the partition components. This eigenvalue optimization problem can be solved by a rearrangement algorithm, which we show to converge in a finite number of iterations to a local minimum of a relaxed objective. I'll also give a consistency result for geometric graphs, stating convergence of graph partitions to an appropriate continuum partition.

Fulkerson Duality for p-Modulus and Applications

Pietro Poggi-Corradini, Kansas State University, pietro@math.ksu.edu

We consider finite graphs $G = (V, E, \sigma)$ with nodes V, edges E, and weights $\sigma \in \mathbb{R}^E_{>0}$. A family of objects Γ on G is identified by a set of vectors N_γ in $\mathbb{R}^E_{>0}$, representing the edge-usage of each object $\gamma \in \Gamma$. To each such family we associate the convex recessive polyhedral set of admissible densities:

$$\text{Adm}(\Gamma) := \left\{\rho \in \mathbb{R}^E_{>0} : N_\gamma^T \rho \geq 1\right\} \subset \mathbb{R}^E_{>0}$$

Given $p \geq 1$, the modulus $\text{Mod}_{p,\sigma}(\Gamma)$ is the minimum energy $E_{p,\sigma}(\rho) = \sum_{e \in E} \sigma(e)\rho(e)^p$, for densities ρ in $\text{Adm}(\Gamma)$. The Fulkerson dual family for Γ is the set $\hat{\Gamma} := \text{ext}\big(\text{Adm}\,(\Gamma)\big) \subset \mathbb{R}^E_{>0}$ consisting of the extreme points of $\text{Adm}(\Gamma)$. The modulus of $\hat{\Gamma}$ is essentially the reciprocal of Γ 's:

$$\text{Mod}_{p,\sigma}(\Gamma)^{\frac{1}{p}}\, \text{Mod}_{q,\sigma^{-\frac{q}{p}}}\big(\hat{\Gamma}\big)^{\frac{1}{q}} = 1,$$

where q is the Hölder conjugate exponent of p. Moreover, the optimal $\rho^* \in \text{Adm}(\Gamma)$ and $\eta^* \in \text{Adm}(\hat{\Gamma})$ satisfy:

$$\eta^*(e) = \frac{\sigma(e)\rho^*(e)^{p-1}}{\text{Mod}_{p,\sigma}(\Gamma)} \quad \forall e \in E$$

In this talk we will discuss four applications of this theory related to the probabilistic interpretation of modulus; a new proof that effective resistance is a metric; monotonicity with respect to edge-conductances; Lovasz-type inequalities on graphs with random weights σ.

Graphs versus Metric Graphs, and First Order Analysis in Metric Spaces
Nageswari Shanmugalingam, University of Cincinnati, shanmun@uc.edu

The traditional way of looking at graphs is to think of it as a pair of sets, the first the set of vertices and the second the adjacency relations (edges). In this talk we will see how to turn this into a metric graph, and apply the tools from first order analysis in metric spaces to such a graph setting.

Analysis and Design of Robust and High-Performance Complex Dynamical Networks
Milad Siami, Massachusetts Institute of Technology, siama@mit.edu

The interest in performance and robustness analysis of large-scale dynamical network is rapidly growing. Improving global performance as well as robustness to external disturbances in large-scale dynamical networks are crucial for sustainability, from engineering infrastructures to living cells; examples include a group of autonomous vehicles in a formation, interconnected transportation networks, cloud-based services, energy and power networks, metabolic pathways and even financial networks. We first show the foundational role of underlying graph of consensus networks in the emergence of several theoretical hard limits on the global performance and robustness of networks. We then introduce the notion of systemic measures for linear consensus networks. Several existing and widely used performance measures in the literature are in fact special cases of this class of systemic measures. Next, we show that for a given linear consensus network and a systemic measure, several strategies can be employed to optimize the network performance. We finally discuss the problem of approximating a given dense consensus network by a suitable sparse network and propose an efficient and fast algorithm for finding a near-optimal sparse approximation of a given network.

Identification of Missing Links Using Susceptible-Infected-Susceptible Epidemic Traces
Aram Vajdi, Kansas State University, avajdi@ksu.edu

The study of Susceptible-Infected-Susceptible (SIS) epidemics on networks has stressed the role of the network topology on the spreading process. However, accurate models of SIS epidemics rely on the complete knowledge of the network topology, which is often not available. Here we tackles the problem of inferring the network topology from observed infection time traces, especially where the network topology is partially known or known with some uncertainty. We propose a Bayesian method to infer the posterior probability of uncertain links in the network, and we derive closed form equations for these probabilities. We also propose a numerical approach based on a Gibbs sampling when the number of uncertain links is large such that using the closed form equations becomes impractical. Numerical results show the capability of the proposed approach to assign high probability to existing links and low probability to non-existing links of the network when the SIS traces are sufficiently long. This is a joint work with Caterina Scoglio.

An Approach to Quad Meshing Based on Harmonic Cross-Valued Maps and the Ginzburg-Landau Theory
Ryan Viertel, University of Utah, rdviertel@gmail.com

A generalization of vector fields, referred to as N-direction fields or cross fields when N = 4, has been recently introduced and studied for geometry processing, with applications in quadrilateral meshing, texture mapping, and parameterization. We observe that cross field design for two-dimensional quad meshing is related to the well-known Ginzburg-Landau problem. This identification yields a variety of theoretical tools for efficiently computing boundary-aligned quad meshes, with provable guarantees on the resulting mesh, for example, the number of mesh defects and bounds on the defect locations. The procedure for generating the quad mesh is to (i) find a complex-valued representation field that minimizes the Dirichlet energy subject to a boundary constraint, (ii) convert the representation field into a boundary-aligned, smooth cross field, (iii) use separatrices of the cross field to partition the domain into four sided regions, and (iv) mesh the four-sided regions using standard techniques. We prove that this procedure can be used to produce a cross field whose separatrices partition the domain into four sided regions. We use an extension of the Merriman-Bence-Osher threshold dynamics method to minimize the Ginzburg-Landau energy for the optimal representation field. Finally we demonstrate the method on a variety of test domains.

Graph-based Geometrical Data Analysis: Local and Scale-Dependent Dimension
Dominique Zosso, Montana State University, dominique.zosso@montana.edu

Our motivation is a desire to analyze large data sets from a geometric point of view, through a graph-based representation of data points sampled from underlying manifolds. We consider simple graphs and equip the vertex set with a metric (shortest path distance) and a measure (vertex count). We then form balls on the vertex set, and define shells as their boundary sets. We are interested in a notion of dimension relating metric and measure by considering the rate of cluster aggregation: we look at the characteristic exponent relating ball radius to ball volume and shell growth. The resulting definitions provide several flavors of cluster growth dimension on the graph, that are both local and scale dependent. We now propose to use this concept of local and scale-dependent dimension towards the development of d-critical balls (the largest ball around a vertex at rate-exponent d) and d-maximal balls (d-critical ball not included in any other d-critical ball). These derived concepts will eventually serve the definition of medial vertices as used in skeletons in mathematical morphology, and boundary vertices. We present preliminary results on random geometric graphs, Cartesian graphs, percolated Cartesian graphs, and some fractal graphs.

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MS16 "Analysis, Computation, and Applications of PDE"

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A Hybrid Method for Stiff Reaction-diffusion Equations

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For stiff reaction-diffusion equations, the semi-implicit integration factor method (IIF) is effective due to its nice stability condition. IIF was previously designed for systems in which the reactions contain no explicitly time-dependent terms and the boundary conditions are homogeneous. For the explicitly time-dependent reaction terms, we find IIF-like methods require small time steps to achieve the theoretical order of accuracy. Although the implicit exponential time differencing (iETD) method can accurately handle the explicitly time-dependent reactions, it is more computationally expensive when solving systems with explicitly time-independent terms. In this study, we develop a hybrid approach that takes advantage of both methods. In this method, IIF is applied to reaction terms that are not explicitly time-dependent whereas the explicitly time-dependent reactions are dealt with the iETD method. The new hybrid IIF-ETD method (hIFE) is able to achieve the theoretical order of accuracy using large time steps, and can also deal with nonhomogeneous boundary conditions accurately and efficiently. In addition, this approach can be naturally combined with the compact and array representation in IIF or ETD for systems in higher spatial dimensions.

Large Time Step Method for Conservation Laws

Ilija Jegdic, Texas Southern University, ilija.jegdic@tsu.edu

We propose a new version of a finite volume method for approximating solutions of one dimensional hyperbolic conservation laws. With this method we make large time steps and we approach solution at the desired time in less time steps. The approximating solutions satisfy the Kruzkov entropy condition in the case of a scalar equation. We also present numerical simulations for Burger's equation and for the Lax shock tube problem for Euler gas dynamics equations.

Weak Galerkin Finite Element Methods and Numerical Applications

Lin Mu, Oak Ridge National Laboratory, mul1@ornl.gov

Weak Galerkin FEMs are new numerical methods that were first introduced by Wang and Ye for solving general second order elliptic PDEs. The differential operators are replaced by their weak discrete derivatives, which endows high flexibility in developing high order numerical schemes on the polytonal meshes. This new method is a discontinuous finite element algorithm, which is parameter-free, symmetric, and absolutely stable. Furthermore, through the Schur-complement technique, an effective implementation of the WG is developed. Several applications of weak Galerkin methods will be discussed in this talk.

Interior Penalty Discontinuous Galerkin Finite Element Methods for Linear Elliptic PDEs in Non-divergence Form

Stefan Schnake, The University of Oklahoma, schnake@math.utk.edu

This talk will focus on discontinuous Galerkin methods to approximate strong solutions for linear elliptic PDEs in non-divergence form whose coefficients are only continuous. These PDEs present themselves in the nonlinear Hamilton-Jacobi-Bellman equations, which have applications in stochastic optimal control and mathematical finance, as well as the linearization of the Mange-Amprere equations. We introduce a few interior penalty, discontinuous Galerkin, finite element methods which are simple in construction. The highlight of the talk will be to show the stability of these methods through a discrete Calderon-Zygmund estimate. Several numerical tests will be shown towards the end of the talk. This talk is based on a joint work with Xiaobing Feng of the University of Tennessee and Michael Neilan of the University of Pittsburgh.

Mean Ages for a Terrestrial Carbon Dynamics Model

Ying Wang, University of Oklahoma, wang@ou.edu

In this talk, I will introduce a nine-dimensional non-autonomous compartmental system modeling the terrestrial carbon cycle. I will define a non-autonomous version of transit time as the mean age of mass leaving the compartmental system at a particular time and show that our non-autonomous theory generalizes the autonomous case. I will apply these results to study the nine-dimensional non-autonomous carbon cycle compartmental model. I will demonstrate that the non-autonomous versions of transit time and mean age differ significantly from the autonomous quantities when calculated for that model.

Local Discontinuous Galerkin Methods for the Coupled BBM-BBM System

Yulong Xing, Ohio State University, xing.205@osu.edu

Nonlinear, dispersive wave equations arise in a number of important application areas. The coupled BBM-BBM system describes the small-amplitude long waves on the surface of water in a channel. In this talk, we present local discontinuous Galerkin methods with both conservative and dissipative numerical fluxes to solve the coupled BBM-BBM system. Numerical examples are shown to establish accuracy and stability of the method, including generation of soliton waves and head-on collisions of solitary waves.

Nonlinear Diffusion Equations with Orientated Convection

Hailong Ye, Shenzhen University, yhl@szu.edu.cn

In this talk, we discuss non-Newtonian polytropic filtration equation with orientated convection, by paying attention to some properties of solutions such as the one of finite propagation of perturbations, and the one of instantaneous shrinking of supports, etc.

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MS17 "Dynamical Systems – Theory and Applications"

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Young Tower and Thermodynamic Formalism for Hyperbolic Systems with Singularities

Jianyu Chen, University of Massachusetts Amherst, jchen@math.umass.edu

This is a joint work with Fang Wang and Hong-Kun Zhang. In this paper, we investigate the chaotic billiards and other related hyperbolic systems with singularities, and construct a special Young tower whose first return to the base is proper. This leads to a Markov partition of the phase space with countable states. Based on such special Young tower structure, we further establish the thermodynamic formalism for the family of geometric potentials, by adapting the inducing scheme framework developed by Pesin, Senti and Zhang. Stochastic properties of the corresponding equilibrium measures immediately follow, including the existence and uniqueness, the decay rates of correlations and the central limit theorem. All the results apply to Sinai dispersing billiards, and their small perturbations due to external forces and nonelastic reflections with kicks and slips.

No-slip Billiards in Three Dimensions

Chris Cox, University of Delaware

We investigate the dynamics of no-slip billiards, a model in which small rotating disks may exchange linear and angular momentum at collisions with the boundary. In particular, we extend boundedness results known in dimension two and consider the extension of the measure preservation property of the no-slip map to higher dimensions. Examples suggest that the ubiquitous obstructions encountered while attempting to construct two dimensional no-slip billiards may be far less common in dimension three. This is a joint work with Renato Feres, Tim Chumley, and Scott Cook.

Billiard Models, Averaging, and Transport Problems

Alex Grigo, University of Oklahoma, grigo@math.ou.edu

In this talk I will present billiard models that arise in certain models of interacting particle systems. The aim of the talk will be to give an overview of existing results for various transport phenomena, and to describe an averaging theorem for such hyperbolic systems with singularities that allows to derive one such transport law.

On Rigidity of Circle Diffeomorphisms with Breaks and Generalized Interval Exchange Transformations

Sasa Kocic, University of Mississippi, skocic@olemiss.edu

I will discuss recent results on rigidity of circle diffeomorphisms with a break (a single point where the derivative has a jump discontinuity) and generalized interval exchange transformations introduced by Marmi, Moussa, and Yoccoz. The theory can be viewed as an extension of Herman's theory on the linearization of circle diffeomorphisms.

Local Limit Theorem for Some Hyperbolic Flows

Peter Nandori, University of Maryland, pnandori@math.umd.edu

We establish the local central limit theorem for some hyperbolic flows. The main ingredient to the proof is the (multidimensional) local central limit theorem for a suitable Poincare map. We will discuss several examples, e.g. suspensions over the Liverani-Saussol-Vaienti maps (including both finite and infinite measure cases), Axiom A flows, Sinai billiards and the geometric Lorenz flow. Based on joint work with D. Dolgopyat.

A Stage-structured Fisher's Equation with Applications in Biochemistry

John Nardini, University of Colorado Boulder, john.nardini@colorado.edu

Recent biological research has sought to understand how biochemical signaling pathways, such as the mitogen-activated protein kinase (MAPK) family, influence the migration of a population of cells during wound healing. Fisher's Equation has been used extensively to model experimental wound healing assays due to its simple nature and known traveling wave solutions. This partial differential equation with independent variables of time and space cannot account for the effects of biochemical activity on wound healing, however. To this end, we derive a structured Fisher's Equation with independent variables of time, space, and biochemical pathway activity level and prove the existence of a self-similar traveling wave solution to this equation. We also consider a more complicated model with different phenotypes based on MAPK activation and numerically investigate how various temporal patterns of biochemical activity can lead to increased and decreased rates of population migration.

Can the Dimension of a Set or Measure Be Inferred from Finite-Dimensional Projections?

William Ott, University of Houston, ott@math.uh.edu

Motivated by infinite-dimensional dynamical systems, we consider how nonlinear projections affect the dimension of a set or measure. Classical results show that when the set lives in a finite-dimensional Euclidean space, Hausdorff dimension is typically preserved. Here we examine the case in which the set lives in a Hilbert or Banach space. Our results hint at the existence of what one might call a "non-computable attractor".

Bistability and Hopf Bifurcation in a Refined Model of HIV Infection

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Recent clinical studies have shown that HIV disease pathogenesis can depend strongly on many factors at the time of transmission, including the strength of the initial viral load and the local availability of CD4+ T-cells. To facilitate these new advances, we will describe a refined in-host model of HIV infection that incorporates the homeostatic proliferation of T-cells. Due to the effects of this biological process, the influence of initial conditions on the proliferation of HIV infection and the dynamics of the model is further elucidated. In particular, our study of the new model extends previous theoretical and computational work on the acute stage of the disease and leads to interesting nonlinear dynamics, including a parameter region featuring bistability of infectious and viral clearance equilibria and the appearance of a Hopf bifurcation within biologically relevant parameter regimes, which may be linked to the appearance of so-called "viral blips".

Stationary Distributions and Convergence Rates for Semistochastic Processes

Nikola Petrov, University of Oklahoma, npetrov@ou.edu

We consider a semistochastic continuous-time continuous-state space random process $\{X(t)\}_{t\geq 0}$ that undergoes downward disturbances of random severity occurring at random times and grows deterministically (governed by an autonomous ODE) between the disturbances. The times of occurrence of the disturbances are distributed according to a Poisson process whose rate $\Lambda(t)$ is allowed to depend on the value of $X(t)$. At each disturbance, the process is multiplied by a continuous random variable (``severity'') supported on $[0,1]$. An important example of such a process is the dynamics of the carbon content of a forest whose deterministic growth is interrupted by natural disasters (fires, droughts, insect outbreaks, etc.).We derive explicit expressions for the stationary distribution of the random process whenever such distribution exists (for an arbitrary ODE and an arbitrary distribution of the severity). The time-dependent distribution of the process $\{X(t)\}_{t\geq 0}$ satisfies an integro-differential PDE. We develop a method for giving an upper bound of the rate at which the distribution of the process at time t approaches the stationary distribution. This is a collaboration with James Broda, Alexander Grigo, and Maria Leite.

Competing Interactions, Patterns, and Traveling Waves in Discrete Systems

Erik Van Vleck, University of Kansas, erikvv@ku.edu

We consider bistable lattice differential equations with competing first and second nearest neighbor interactions. We construct heteroclinic orbits connecting the stable zero equilibrium state with stable spatially periodic orbits of period p=2,3,4 using transform techniques and a bilinear bistable nonlinearity. We investigate the existence, global structure, and multiplicity of such traveling wave solutions. For smooth nonlinearities an abstract result on the persistence of traveling wave solutions is presented and applied to lattice differential equations with repelling first and/or second neighbor interactions and to some problems with infinite range interactions. This talk is based on joint work with Anna Vainchtein (Pittsburgh) and Aijun Zhang (Oregon State).

Specialization Model of Network Growth and its Dynamic Consequences

Ben Webb, Brigham Young University, bwebb@mathematics.byu.edu

One of the characteristics often observed in real networks is that, as a network's topology evolves so does the network's ability to perform complex tasks. To explain this, it has also been observed that as a network grows certain subnetworks begin to specialize the function(s) they perform. We introduce a model of network growth based on this notion of specialization and show that as a network is specialized via this model its topology becomes increasingly modular, hierarchical, and sparser each of which are important properties observed in real networks. Also, as this method of specialization preservers basic spectral properties of a network we are able to show that the network maintains certain dynamic properties, specifically stability, as its structure evolves, under mild conditions, which links specialization to robustness of network function.

Hitting Times Distribution and Extreme Value Laws for Semi-Flows

Fan Yang, University of Oklahoma, fizbanyang@gmail.com

For flows whose return map on a cross section has sufficient mixing property, we show that the hitting time distribution of the flow to balls is exponential in limit. We will also look at the link between the extreme value distribution of the flow and its hitting time distribution.

Homoclinic Intersections for Generic Geodesic Flows on S^2

Pengfei Zhang, University of Oklahoma, pengfei.zhang@ou.edu

We consider the geodesic flow on the two sphere with some Riemannian metric. We showed that for a generic convex metric on S^2, every hyperbolic closed geodesic admits transverse homoclinic intersections.

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MS18 "Model Reduction and Data Assimilation"

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Xuemin Tu, University of Kansas, xuemin@ku.edu

Subspace-based Dimension Reduction: Inputs and Outputs

Paul Constantine, Colorado School of Mines, paul.constantine@mines.edu

Many approaches for reducing the computational costs of complex simulations are based on dimension reduction techniques---in particular, techniques like PCA and POD that exploit low-dimensional subspaces constructed from eigenspaces of particular matrices. I will review subspace-based dimension reduction techniques with an emphasis on distinguishing problems that warrant different choices of methods. In particular, I will compare active subspaces that reduce a model's input (or parameter) space dimension with POD that reduces a model's output (or state) space dimension. And I will compare these approaches to related techniques in statistical learning.

Data Assimilation for Combustion

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Accurate CFD modeling of combustion is expensive and challenging. Data assimilation can help increase the solution accuracy by melding observation with model prediction. However, data assimilation can make it even more expensive. To ensure simulation-assimilation of combustion is feasible, a computationally efficient CFD model is critical. A CFD algorithm has been designed to achieve high accuracy and high performance for combustion simulations. In this talk, numerical features of the data-assimilated CFD algorithm will be discussed. An application of the simulation-assimilation algorithm will be demonstrated for a convection-diffusion-reaction problem.

Optimal Model Reduction of Quadratic Nonlinear Dynamical Systems

Serkan Gugercin, Virginia Tech., gugercin@vt.edu

W extend H2-norm based input-independent, optimal model reduction techniques to an important class of nonlinear systems, namely quadratic-bilinear (QB) dynamical systems. We introduce a truncated H2-norm for QB systems and derive the first-order necessary conditions for an optimal approximation, minimizing the truncated H2-norm. This leads to an iterative model reduction algorithm, which upon convergence yields a reduced-order system that approximately satisfies the derived optimality conditions. We illustrate the efficiency of the proposed method by means of several nonlinear partial differential equations.

Data Assimilation for Geophysical Flows Employing Only Surface Measurements

Michael Jolly, Indiana University, msjolly@indiana.edu

We prove that data assimilation by feedback control can be achieved for the three-dimensional quasi-geostrophic equation using only large spatial scale observables on the dynamical boundary. On this boundary a scalar unknown (buoyancy or temperature of a fluid) satisfies the surface quasi-geostrophic equation. The feedback nudging is done on this 2D model, yet ultimately synchronizes the stream function of the three-dimensional flow. . The main analytical difficulties involved in ensuring the synchronization property arise from the presence of a nonlocal dissipative operator in the surface quasi-geostrophic equation. This necessitates the derivation of various boundedness and approximation properties for the observation operators used in the feedback nudging.

Exploiting Time Scale Separation to Assimilate Lagrangian Data
John Maclean, University of North Carolina at Chapel Hill, jmaclean@email.unc.edu

We are interested in the problem of assimilating information from instruments that drift in the flow in order to estimate ocean flow states. In particular we would like to use data-driven coherent structure methods, that are notably robust under small perturbations of the flow. We take the perspective that the highly nonlinear tracer trajectories are fast, in order to justify computing on a reduced system in which the influence of the drifters is represented by the extracted coherent structure.

Reducing FEM Computations of Eigenvalues via p-Hierarchical Enrichment
Agneiszka Miedlar, University of Kansas, amiedlar@ku.edu

Investigating the behavior of the adaptive finite element eigenvalue and eigenvector algorithms from the point of view of numerical linear algebra (NLA), is the scope of intensive research in the last few years. Several theoretical as well as algorithmic results clearly indicate a real necessity of engaging various NLA techniques into numerical PDE solvers, not only to obtain meaningful and relevant solutions of the real-world problems, but also to encourage the transition from hardware to algorithm oriented computational techniques. In this work, we show that an application of just one implicit inverse iteration step on the computed FEM-Ritz vector not only yields a super-converging Ritz value, but also significantly reduces the cost of underlying finite element computations.

Numerical Approximation of a Feedback-Control Data Assimilation Algorithm: Uniform in Time Error Estimates
Cecilia Mondaini, Texas A&M University, cfmondaini@gmail.com

We consider a feedback-control (nudging) approach for data assimilation that works for a general class of dissipative dynamical systems and observables. The algorithm is defined by modifying the original forecast system through the addition of an extra term which relaxes only the coarse scales of the solution towards the spatially coarse observations. Our goal is to obtain an analytical estimate of the error committed when numerically solving this modified system by using a post-processing technique for the spectral Galerkin method, inspired by the theory of approximate inertial manifolds. This numerical approximation yields a dimensionally reduced version of the modified system. Most importantly, our error estimate is uniform in time, which reflects the global stability of the algorithm. This is a joint work with E. S. Titi.

Accelerating Bayesian Inverse Methods by Approximating Likelihoods as Jagged Random Fields
Gregor Robinson, University of Colorado at Boulder, gregor.robinson@colorado.edu

We show that generalized Gaussian random field models of additive measurement error can accelerate dimensionality-sensitive techniques like MCMC and particle filtering for Bayesian estimation of spatially-extended dynamics. Choosing a ΓÇ£jaggedΓÇ¥ likelihood model, ascribing unboundedly increasing uncertainty in the progression toward short scales, may seem counterintuitive but can acceptably approximate large scale posteriors with significant savings in computational cost. Reducing the rejection sensitivity to diffusion along small-scale subspaces is responsible for this cost improvement. Taking discretized elliptic differential operators as precision matrices provides the desired jagged property of a likelihood model. This choice also introduces structure exploitable by scalable computation techniques, including multigrid solvers. Inverse problems in geophysical fluids often involve measurements from uncontrollable and unpredictable locations, so it is especially convenient that fast solvers are available for the class of elliptic differential operators discretized on nonuniform observation grids.

Sequential Implicit Sampling Methods for Bayesian Inverse Problems
Xuemin Tu, University of Kansas, xuemin@ku.edu

The solution to the inverse problems, under the Bayesian framework, is given by a posterior probability density. For large scale problems, sampling the posterior can be an extremely challenging task. Markov Chain Monte Carlo

(MCMC) provides a general way for sampling but it can be computationally expensive. Gaussian type methods, such as the Ensemble Kalman Filter (EnKF), make Gaussian assumptions even for the possible non-Gaussian posterior, which may lead to inaccuracy. In this talk, the implicit sampling method and sequential implicit sampling method are investigated for the inverse problem involving time-dependent partial differential equations (PDEs). The sequential implicit sampling method combines the idea of the EnKF and implicit sampling and it is particularly suitable for time-dependent problems. Moreover, the new method is capable of reducing the computational cost in the optimization, which is a necessary and the most expensive step in the implicit sampling method. The sequential implicit sampling method has been tested on a seismic wave inversion. The numerical experiments show its efficiency by comparing it with the MCMC and some Gaussian approximation methods.

Projected Data Assimilation and Applications
Erik Van Vleck, University of Kansas, erikvv@ku.edu

In this talk we present a framework for a class of DA techniques based upon a computational time dependent slow/fast splitting. We will discuss advantages and disadvantages of such techniques as well classes of problems for which these techniques are well suited. We outline some specific techniques we have been developing and illustrate their effectiveness through computational results. Finally, we investigate the potential of such techniques for improved uncertainty quantification. Time permitting we will present some applications of these results to a single column radiation-convection model and a land-surface model.

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MS19 "Recent Advances in Numerical PDEs"

Xiaoming He, Missouri University of Science and Technology, hex@mst.edu
Ari Stern, Washington University in St. Louis, stern@wustl.edu
Timo Heister, Clemson University, heister@clemson.edu

An Immersed Finite Element Direct Implicit Particle-in-cell Method for Simulation of Plasmas

Jinwei Bai, Harbin Institute of Technology at Shenzhen, baijinwei@stu.hit.edu.cn

The particle-in-cell (PIC) method has been widely used for plasma simulation, because of its noise-reduction capability and moderate computational cost. The immersed finite element (IFE) method is efficient for solving interface problems on Cartesian meshes, which is desirable for PIC method. The combination of these two methods provides an effective tool for plasma simulation with complex interface/boundary. Direct implicit particle-in-cell method was developed because of that the computational efficiency is significantly increased and the accuracy is maintained, compared with the standard particle-in-cell models. Thus, in this paper, we developed a new method to simulate the motion for plasmas, which combines the immersed finite element method with direct implicit particle-in-cell method. Numerical schemes are discussed and benchmark results are presented. The code can be used to simulate practical ion thrusters.

Fractional Dynamics for Quantum Random Walks

Lucas Bouck, George Mason University, lbouck@gmu.edu

Quantum random walks (QRWs) are important tools for the development of algorithms in the growing field of quantum computing. One interest in studying QRWs is modeling them with partial differential equations (PDEs). This research enriches an available PDE model from Blanchard and Hongler (2004) by including the fractional time derivative. The resulting model is the Fractional Fokker-Planck PDE. We use a spectral method for the spatial derivatives and an L1 finite difference method for the fractional time derivative to compute a numerical solution to this PDE. We also developed an algorithm to find the optimal order of the fractional time derivative to best fit the discrete QRW.

Practical and Efficient Time Integration and Kronecker Product Solvers

Jed Brown, University of Colorado at Boulder, jed.brown@colorado.edu

Most time integrators for large-scale problems, such as semi-discretized partial differential equations, solve one stage at a time. When stage equations involve solution of linear systems represented using sparse matrices, this invariably results in poor hardware utilization due to low arithmetic intensity and poor vectorization. Implicit Runge-Kutta (IRK) methods solve coupled systems involving all stages in a step, and in turn benefit from excellent accuracy and stability properties as well as optional symplecticity. While quite successful in the dense and research ODE communities, IRK has only recently received attention from the PDE community, but using solution methods for which total work grows superlinearly in number of stages and each stage suffers from the same attributes that produce low efficiency for sequential stepping. In this work, we investigate practical and efficient multilevel solution algorithms for such Kronecker product systems on modern parallel architectures. These methods offer convenient vectorization and high arithmetic intensity similar to multiple right hand sides, along with improved strong scaling due to reduced communication requirements. We will also draw connections with a formulation derived from exponential integrators that circumvents an eigenbasis ill-conditioning issue that has plagued other efforts.

An Explicit Posteriori Error Estimations for the Cell Functional Minimization Scheme of Elliptic Problems
Yanzhao Cao, Auburn University, yzc0009@auburn.edu

We present an explicit form of a posteriori error estimator for the cell functional minimization discrete scheme of elliptic problems. We show that this estimator is reliable with respect to an energy-type error. The performance of the error indicator in the adaptive mesh refinement algorithm is investigated, by numerically solving the diffusion equation on computational domains with different types of computational meshes.

Discrete Unified Gas Kinetic Scheme with a Force Term for Micro-channel Flows
Yong Cao, Harbin Institute of Technology at Shenzhen, yongc@hit.edu.cn

In this paper a discrete unified gas kinetic scheme (DUGKS) with a force term is developed for micro-channel flows, which is mostly the low-speed isothermal flow. The direct discretization and indirect discretization of force scheme are discussed, and the result show the indirect discretization scheme is more suitable for low-speed isothermal flow. To accurately realize the pressure boundary condition, a linear extrapolation scheme is also introduced. In this study, the external force driven and pressure driven micro-channel flows have been investigated by DUGKS. The numerical results, including the velocity profile and the mass flow rate, as well as the nonlinear pressure distribution along the channel, agree fairly well with the solutions of the linearized Boltzmann equation, the direct simulation Monte Carlo results, the experimental data. In addition, the present results of the velocity profile show that DUGKS can gain an accurate simulation for the micro-channel gas flow with all Knudsen numbers.

A Finite Element Framework for Flexible and Adaptive Geometric Multigrid
Timo Heister, Clemson University, heister@clemson.edu

We present data structures and implementation details of a geometric multigrid method on adaptively refined meshes for massively parallel finite element computations. The method uses local smoothing on the refined part of the mesh. Partitioning is achieved by using a space filling curve for the leaf mesh and distributing ancestors in the hierarchy based on the leaves. The method is flexible and shown to work with continuous, DG, and mixed elements of arbitrary order and is scaling to 10,000 cores and more than one billion DoFs. The algorithm is implemented as part of the deal II finite element library and as such available to the public.

Elastodynamics Coupling over Non-coincident Interfaces
Paul Kuberry, Sandia National Laboratories, pakuber@sandia.gov

When complex geometric domains are decomposed into subdomains that are discretized independently, the interfaces between the subdomains can have mismatched nodes and even non-coincident surfaces with gaps and overlaps. Constructing algorithms to couple the subdomain problems in a way that will satisfy the interface conditions on the subdomains ΓÇÖ boundaries and also preserve accuracy and stability is a challenging problem. We describe the construction of a virtual interface and associated operators, which map solutions to and from subdomain interfaces. Additionally, we develop operators useful for mapping a single function to two distinct subdomain interfaces in a manner that preserves global flux conservation. We use these tools to generalize conventional Lagrange multiplier formulations of the governing equations on non-overlapping subdomains to obtain a mixed formulation of these equations for general interface configurations, including non-coincident interfaces. We then derive a generalization of the dual Schur complement approach, which leads to a partitioned scheme for the governing equations. We provide the results of numerical experiments demonstrating successfully passing a pass test, optimal convergence rates, and global flux conservation.

Numerical Approximation of the Stokes-Biot system
Hyesuk Lee, Clemson University, hklee@clemson.edu

Computational algorithms for the Stokes-Biot coupled system are proposed for the interaction of a free fluid with a poroelastic structure. The talk is focused on a decoupling scheme that allows the Stokes and Biot systems solved independently. The decoupling strategy is to cast the coupled fluid-poroelastic system as a constrained optimization problem with a Neumann type control that enforces continuity of the normal components of the stress on the interface. The optimization objective is to minimize any violation of the other interface conditions. Numerical algorithms based on a residual updating technique are discussed and numerical results are provided to validate the accuracy and efficiency of the proposed algorithms.

Discontinuous Galerkin Method for Solving a Thin-film Equation
Caleb Logemann, Iowa State University, logemann@iastate.edu

Aircraft icing is a critical operational, safety, and certification concern for the aircraft industry. Aircraft icing occurs in regimes that involve residual surface water that is transported along the surface, also known as runback. The water mass transport or runback can be modeled using thin-film equations. The thin-film equation results from an asymptotic limit of the Navier-Stokes equations. The thin-film equation contains both a nonlinear hyperbolic transport and nonlinear parabolic diffusion terms. Generally, these terms are handled separately using operator splitting. We describe how to use an explicit Runge-Kutta DG method for solving the nonlinear hyperbolic equation and an implicit DG method for solving the nonlinear parabolic diffusion equation. To ensure fast convergence of the implicit method a multi-grid approach is used.

Bayesian Method for Inverse Problem with Uncertainty Quantification
Ju Ming, Huazhong University of Science and Technology, Jming@hust.edu.cn

In this talk, several inverse problems governed by stochastic PDEs will be presented. A Bayesian-based approach was introduced to reduce the uncertainty. Numerical tests were performed to verify our method.

Stochastic Inverse Problems for Multiscale Computation
Nishant Panda, Colorado State University, nishant.panda@gmail.com

Descriptions of complex multiscaled physical systems often involve many physical processes interacting through a multitude of scales. In many cases, the primary interest lies in predicting behavior of the system at the macroscale (i.e., engineering scale) where continuum, physics-based, models such as partial differential equations provide high fidelity descriptions. However, in multiscale systems, the behavior of continuum models can depend strongly on microscale properties and effects, which are often included in the macroscale model as a parameter field obtained by some upscaling process from a microscale model. Generally, a number of choices have to be made in choosing an upscaling procedure and the resulting representation of the parameter. These choices have a strong impact on both the fidelity and the computational efficiency of the model. Thus, choosing a good parameter representation and upscaling procedure becomes part of the uncertainty quantification and prediction problem for a multiscale model. We consider the use of output data from the macroscale model to formulate and solve a stochastic inverse problem to determine probability information about the upscaled parameter field. In particular, we extend a measure-theoretic inverse problem framework and non-intrusive sample-based algorithm to determine the choices of parameter representation and upscaling procedure that are most probable given uncertain data from the macroscale model. We illustrate the methodology in the context of shallow water flow and sub-surface flow.

Uniqueness of Discrete Solutions to Quasilinear PDE
Sara Pollock, Wright State University, sara.pollock@wright.edu

We will discuss a discrete comparison principle for a class of nonmonotone quasilinear partial differential equations, discretized by piecewise linear finite elements. The comparison principle implies the uniqueness of the solution to the discrete problem. We establish that without the presence of lower-order terms, a globally small mesh size is not required. It is sufficient for the mesh size to be locally controlled, based on the variance of the solution over each element, essentially requiring the mesh to be fine where the gradient is steep.

A Multi-Physics Domain Decomposition Method for Navier-Stokes-Darcy Model
Changxin Qiu, Missouri University of Science and Technology, cqrg7@mst.edu

In a karst aquifer, free flow and porous media flow are tightly coupled together, for which the Navier-Stokes-Darcy model has higher fidelity than either the Darcy or Navier-Stokes systems on their own. The Stokes-Darcy type model has attracted significant attention in the past ten years. However, coupling the two constituent models leads to a very complex system. This presentation discusses a multi-physics domain decomposition method for solving the Navier-Stokes-Darcy system. Computational results are presented to illustrate the features of the proposed method.

Symplectic Hamiltonian HDG Methods for Wave Propagation Phenomena
Manuel Sanchez, University of Minnesota, sanchez@umn.edu

We devise the first symplectic Hamiltonian hybridizable discontinuous Galerkin (HDG) methods for the acoustic wave equation. We discretize in space by using a Hamiltonian HDG scheme, that is, an HDGmethod which preserves the Hamiltonian structure of the wave equation and in time by using symplectic, diagonally implicit and explicit partitioned Runge-Kutta methods. The fundamental feature of the resulting scheme is that the conservation of a discrete energy, which is nothing but a discrete version of the original Hamiltonian, is guaranteed. We present numerical experiments which indicate that the method achieves optimal approximations of order $k+1$ in the L^{2}-norm when polynomials of degree $k\geq0$ and Runge-Kutta time-marching methods of order $k+1$ are used. In addition, by means of post-processing techniques and by increasing the order of the Runge-Kutta method to $k+2$, we obtain super convergent approximations of order $k+2$ in the L^2-norm for the displacement and the velocity.

Multisymplecticity of Finite Element Methods for Hamiltonian PDEs
Ari Stem, Washington University in St. Louis, stern@wustl.edu

I will discuss some recent work with Robert McLachlan on finite element methods (specifically HDG methods) that preserve the multisymplectic conservation law for Hamiltonian PDEs. In particular, we introduce notions of "weak" and "strong" multisymplecticity for a method and show how this distinction is related to conservativity of numerical fluxes.

A Positivity-preserving Numerical Scheme for the Cahn-Hilliard Equation with Logarithmic Potential
Cheng Wang, University of Massachusetts Dartmouth, cwang1@umassd.edu

The Cahn-Hilliard model with logarithmic potential is considered, in which the key difficulty has always been associated with the singularity of the logarithmic terms. An energy stable scheme, which implicitly treats the logarithmic terms, is proposed and analyzed in this talk. In particular, how to ensure the bound of the numerical solution in the interval of (0,1), so that the numerical scheme is well-defined at a point-wise level, has been a long-standing mathematical challenge. It is proved that, given any numerical solution with a fixed bound in maximum norm, there exists a unique numerical solution that satisfies the given bound (0,1) at a point-wise level. As a result, the numerical scheme is proven to be well-defined, and the unique solvability and energy stability could be established with the help of convexity analysis. Some numerical results are also presented in the talk.

Thermo-acoustic Tomography in an Inhomogeneous Medium with Planar Detectors

Yang Yang, Michigan State University, yangy5@msu.edu

Thermo-acoustic tomography is a hybrid medical imaging modality where optical waves and ultrasound waves are coupled. The propagation of ultrasound waves is typically modeled as an inverse source problem for the acoustic wave equation. In this talk we discuss this inverse source problem in an inhomogeneous medium where the wave speed is variable and the measurement is made by large planar detectors. We prove uniqueness and stability on the recovery of the source with full or partial boundary measurement, and give procedures to reconstruct the singularities of the source. This is joint work with Plamen Stefanov from Purdue University.

Superconvergence of HDG Methods for Convection-diffusion Equations

Huiqing Zhu, University of Southern Mississippi, huiqing.zhu@usm.edu

We study the nodal superconvergence of hybridizable LDG methods (LDG-H) for one-dimensional convection-reaction-diffusion problems. We found that the LDG-H approximations to the solution and its derivative superconverge at mesh nodes and certain interior points when the stabilization parameters are properly chosen. We also compared these results with the superconvergence of Finite Element Method (FEM) and some Discontinuous Galerkin methods (DG).

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MS20 "Numerical Methods for Multi-physics Problems"

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Accurate Solution of Flow Problems for the Earth Mantle

Wolfgang Bangerth, Colorado State University, bangerth@colostate.edu

On long enough time scales, the Earth mantle behaves like a vigorously convecting fluid. It can adequately be described by Stokes flow coupled to an advection diffusion equation for the temperature. The primary difficulty is that all coefficients in these equations -- and in particular the viscosity -- are strongly dependent on the temperature and can vary by orders of magnitude, often discontinuously. This presents significant difficulties to discretizations and solvers. This talk will detail these difficulties and present approaches to address them.

Splitting up Method for the 2D Stochastic NavierΓÇôStokes Equations

Hakima Bessaih, University of Wyoming, bessaih@uwyo.edu

We investigate the convergence of an iterative scheme for the 2-d stochastic Navier-Stokes equations on the torus suggested by the Lie-Trotter product formulas for stochastic differential equations of parabolic type. The stochastic system is split into two problems which are simpler for numerical computations. An estimate of the approximation error is given for periodic boundary conditions. In particular, we prove that the strong speed of the convergence in probability is almost 1/2, by localizing on a set of arbitrary large probability.

A Finite Element Method Perturbation Expansion for a Coupled 2D Structural-Acoustic System

Li Deng, University of Wyoming, lisa.deng68@gmail.com

The structural acoustic coupled vibration problem is very important in many engineering applications such as quality control of vehicles. Formulating the problem using the finite element method leads to a nonsymmetric generalized eigenvalue problem. We show that the problem can be reformulated into uncoupled structural and acoustic problems by introducing a coupling strength parameter ε as a multiplier applied to the off-diagonal coupling terms. The discretized uncoupled problems then lead to a pair of symmetric generalized eigenvalue problems which can be efficiently and independently solved. The solutions of the uncoupled problems are then used to compute the coupled solution using the perturbation method and the introduced coupling strength parameter. We confirm the adequacy of the method by investigating numerical examples for a two dimensional uniform mesh, whose exact solution is known, as well as arbitrary meshes for a car-like example.

GPU Accelerated Sequential Quadratic Programming

Craig Douglas, University of Wyoming, craig.c.douglas@gmail.com

Nonlinear optimization problems arise in all industries. Accelerating optimization solvers is desirable. Efforts have been made to accelerate interior point methods for large scale problems. However, since the interior point algorithm used requires many function evaluations, the acceleration of the algorithm becomes less beneficial. We introduce a way to accelerate the sequential quadratic programming method, which is characterized by minimizing function evaluations, on graphical processing units.

A Decoupled Unconditionally Stable numerical Method for Solving the Cahn-Hilliard-Stokes-Darcy Phase Field System

Daozhi Han, Missouri University of Science and Technology, daozhih@gmail.com

In this talk, we present a decoupled numerical scheme for solving the Cahn-Hilliard-Stokes-Darcy model for two-phase flows in karstic geometry. In the numerical scheme, we explore a fractional step method to decouple the phase-field (Cahn-Hilliard equation) from the velocity field (Stokes-Darcy fluid equations). To further decouple the Stokes-Darcy system, we introduce a first order pressure stabilization term in the Darcy solver so that the Stokes system is decoupled from the Darcy system. We show that the scheme is uniquely solvable, energy stable, and mass conservative. This work is joint with Wenbin Chen and Xiaoming Wang.

Numerical Simulation of 2D Unsteady Shear-Thinning Non-Newtonian Incompressible Fluid in Screw Extruder with Fictitious Domain

Qiaolin He, Sichuan University, qlhejenny@scu.edu.cn

In this talk, we develop a fictitious domain method with Distributed Lagrange Multipliers for simulating 2D unsteady shear-thinning non-newtonian incompressible flow in a single-screw and twin-screw extruder. The advantage of the fictitious domain method is that one can use a fixed mesh even as the fluid domain changes in time (as the screws are rotating), eliminating the need for repeated re-meshing and projection. The method uses a finite element discretization in space and an operator-splitting technique for discretization in time. Numerical results are given for the flow inside a single-screw extruder or twin-screw extruder, which show the fictitious domain method is efficient for the problem.

Numerical Renormalization Group Algorithms for Self-similar Solutions of Partial Differential Equations

Long Lee, University of Wyoming, llee@uwyo.edu

We introduce and systematically investigate a numerical procedure that reveals the asymptotically self-similar dynamics of solutions of partial differential equations (PDEs). The approach is based on the renormalization group (RG) theory for PDEs. This numerical version of RG method, dubbed as the numerical RG algorithm, numerically rescales the temporal and spatial variables in each iteration and drives the solutions to a fixed point exponentially fast, which corresponds to self-similar dynamics of the equations. Moreover, the procedure allows us for detecting and further finding the critical exponent of the logarithmic decay hidden in self-similar solutions. We carefully examine the ability of the algorithm for determining the critical scaling exponents in time and space that render explicitly the distinct physical effects of the solutions of the Burgers equation, depending on the initial conditions. We use the phenomena of dispersive shock waves of the Korteweg-de Vries equation to show that the algorithm can be used as a time integrator for investigating intermediate asymptotic behavior of solutions. Finally, we illustrate the ability of the numerical RG procedure for detecting and capturing the hidden logarithmic decay through a nonlinear system of cubic autocatalytic chemical reaction equations.

Immersed Finite Element Time Domain Methods for Maxwell Equations in Complex Media

Chang Lu, Harbin Institute of Technology, Shenzhen Graduate School, luchang@stmail.hitsz.edu.cn

This paper developed an immersed finite element time domain (IFETD) method to solve the Maxwell equations in complex media. This problem arise from electromagnetic scattering and radiation simulation in composite materials. A structured mesh can be used in this IFETD method to simulate 2-D scattering and radiation in a domain with complex interfaces separating different materials, this method provides a new way to study the motion of plasma in time varying electromagnetic field. Numerical examples are provided to demonstrate that the accuracies of these IFE methods are comparable to the standard finite element method with unstructured body-fit mesh.

Coupled Fire-atmosphere-fuel Moisture-smoke Online Modeling with WRF-SFIRE
Jan Mandel, University of Colorado at Denver, jan.mandel@ucdenver.edu

Jan Mandel, University of Colorado Denver; Adam Kochanski, University of Utah; Sher Schranz, NOAA/CIRA Martin Vejmelka, AVAST. We present an integrated wildland fire model based on combining a high resolution, multi-scale weather forecasting model WRF, with a semi-empirical fire spread model, dead fuel moisture model, and chemical smoke transport model. The fire-released heat and moisture impact local meteorology. The fuel moisture model is driven by the atmospheric component of the system. The wind and the fuel moisture in turn impact the fire rate of spread. Fire emissions are input into the atmospheric model as tracers or in the coupled chemistry model WRF-Chem. The fire simulations are initialized by a web-based control system allowing a user to define a fire as well as basic simulation properties such as simulation length, type of meteorological forcing and resolution, anywhere in CONUS and any time meteorological products are available. The data is downloaded automatically, and the system monitors execution on a cluster. The simulation results are processed while the model is running and displayed in a visualization portal at http://demo.openwfm.org This research was partially supported by NASA grant NNX13AH59G.

A Stabilized Dual Mixed Hybrid Finite Element Method for Three-Dimensional Transmission Problems
Aurelio Giancarlo Mauri, University Politecnico Milano, aureliogiancarlo.mauri@polimi.it

In the present work we propose a novel dual mixed hybrid (DMH) finite element method (FEM), based on the Raviart-Thomas finite element space of lowest order, for the numerical approximation of a boundary value problem with diffusive, advective and reactive terms to be solved in a three-dimensional domain with transmission conditions across a selective interface. The novelty of the formulation consists of the introduction of (1) a pair of Lagrange multipliers, as in the Three-Field method, to account for the presence of the interface and (2) an artifical diffusion in the streamline direction, as in the SUPG method, to stabilize the computation against advection dominance. A theoretical error analysis shows that the scheme enjoys optimal convergence properties with respect to the finite element discretization parameter. Extensive computational tests demonstrate the theoretical conclusions and indicate that the proposed DMH FEM method is accurate and stable even in the presence of marked interface jump discontinuities of both solution and associated normal flux. Results also show that in the case of strongly dominating advective terms, the proposed method is capable to accurately resolve steep boundary and/or interior layers without introducing spurious unphysical oscillations or excessive smearing of the solution front.

A Locally Conservative Stabilized Continuous Galerkin Finite Element Method for Two-Phase Flow in Poroelastic Subsurfaces
Bradley McCaskill, University of Wyoming, bmccaski@uwyo.edu

We study the application of a stabilized continuous Galerkin finite element method (CGFEM) in the simulation of multiphase flow in poroelastic sub-surfaces. The system involves a nonlinear coupling between the fluid pressure, subsurface's deformation, and the fluid phase saturation, and as such, we represent this coupling through an iterative procedure. Spatial discretization of the poroelastic system employs the standard linear finite element in combination with a numerical diffusion term to maintain stability of the algebraic system. Furthermore, direct calculation of the normal velocities from pressure and deformation does not entail a locally conservative field. To alleviate this drawback, we propose an element based post-processing technique through which local conservation can be established. The performance of the method is validated through several examples illustrating the convergence of the method, the effectivity of the stabilization term, and the ability to achieve locally conservative normal velocities. Finally, the efficacy of the method is demonstrated through simulations of realistic multiphase flow in poroelastic subsurfaces.

UKF-GMMR Approach for Fault Detection and Diagnosis
Liping Wang, University of Wyoming, lwang12@uwyo.edu

This study presents a novel data-driven approach for automated fault detection and diagnosis for a multi-chiller plant. Gaussian Mixture Model Regression (GMMR) algorithm is used to model the chiller plant based on measurement data. Unscented Kalman Filter (UKF) is integrated into GMMR for adjusting the model parameters based on the feedback of residual between observation and model prediction. The proposed algorithm is able to detect and diagnose simultaneous faults in the system by monitoring variations of key GMMR parameters.

A Spectral Projection Preconditioner for Solving Ill Conditioned Linear Systems

Man-Chung Yeung, University of Wyoming, myeung@uwyo.edu

We present a preconditioner based on spectral projection that is combined with a deflated Krylov subspace method for solving ill conditioned linear systems of equations. Our results show that the proposed algorithm requires many fewer iterations to achieve the convergence criterion for solving an ill conditioned problem than a Krylov subspace solver. In our numerical experiments, the solution obtained by the proposed algorithm is more accurate in terms of the norm of the distance to the exact solution of the linear system of equations.

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MS21 "Recent Developments in Discontinuous Galerkin Methods for Partial Differential Equations"

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Jue Yan, Iowa State University, jyan@iastate.edu

A Stochastic Local Discontinuous Galerkin Method for Stochastic Boundary-value Problems Driven by Additive Noises

Mahboub Baccouch, University of Nebraska at Omaha, mbaccouch@unomaha.edu

The local discontinuous Galerkin (LDG) method has been successfully applied to deterministic boundary-value problems (BVPs) arising from a wide range of applications. In this talk, we propose a stochastic analogue of the LDG method for stochastic BVPs. We first approximate the white noise process by a piecewise constant random process to obtain an approximate BVP. We show that the solution of the new BVP converges to the solution of the original problem. The new problem is then discretized using the LDG method for deterministic problems. We prove that the solution to the new approximate BVP has better regularity which facilitates the convergence proof for the proposed LDG method. More precisely, we prove error estimates for the solution and for the auxiliary variable that approximates the first-order derivative in the mean-square sense. We also apply a stochastic analogue of the deterministic LDG method to the heat and wave problems driven by additive noises. Numerical experiments are performed to show the robustness of our proposed schemes. Finally, several numerical examples are provided to illustrate the theoretical results.

An HDG Method for a Distributed Optimal Control Problem

Fatih Celiker, Wayne State University, celiker@wayne.edu

We present a priori error analysis of a hybridizable discontinuous Galerkin (HDG) method for a distributed optimal control problem governed by diffusion equations. The error estimates are established based on the projection-based approach recently used to analyze these methods for the diffusion equation. We prove that for approximations of degree k on conforming meshes, the orders of convergence of the approximation to fluxes and scalar variables are $k+1$ when the local stabilization parameter is suitably chosen.

Optimally Convergent HDG Method for Fifth-Order Korteweg-de Vries type Equations

Bo Dong, University of Massachusetts Dartmouth, bdong@umassd.edu

We develop and analyze the first hybridizable discontinuous Galerkin (HDG) method for solving fifth-order Korteweg-de Vries type equations. The approximate solutions are defined by a discrete version of a characterization of the exact solution in terms of the solutions to local problems on each element which are patched together through transmission conditions on element interfaces. We prove that the semi-discrete scheme is stable with proper choices of stabilization function in the numerical traces. For the linearized equation, we show that the approximations to the exact solution and its derivatives have optimal convergence rates. In numerical experiments, we use implicit schemes for time discretization and the Newton-Raphson method for solving nonlinear equations, and we observe optimal convergence rates for both the linear and the nonlinear fifth-order equations.

Divergence-conforming HDG Methods for the Brinkman Equations

Guosheng Fu, Brown University, guosheng_fu@brown.edu

We present new parameter-free superconvergent H(div)-conforming HDG methods for the Brinkman equations on both simplicial and rectangular meshes. We obtain optimal error estimates in L2 norms for all the variables in both the Stokes-dominated regime (high viscosity/permeability ratio) and Darcy-dominated regime (low viscosity/permeability ratio). We also obtain superconvergent L2 estimate of one order higher for a suitable projection of the velocity error, which is typical for (hybrid) mixed methods for elliptic problems. Moreover, thanks to H(div)-conformity of the velocity, our velocity error estimates are independent of the pressure regularity.

High Degree Immersed Finite Element Spaces by a Least Squares Method based on Fictitious Elements

Ruchi Guo, Virginia Tech, ruchi91@vt.edu

We present a least squares framework for constructing p-th degree immersed finite element (IFE) spaces for solving typical second-order elliptic interface problems. The IFE shape functions are constructed on fictitious elements to improve the conditioning of the linear system resulted in the least square formulation. The jump conditions are weakly satisfied by minimizing a penalty along the interface inside each fictitious elements, which naturally guarantees the existence of IFE shape functions on each interface element of an interfaced independent mesh.

Solvers for Interfaces Problems with Unfitted Meshes

Marcus Sarkis, Worcester Polytechnic Institute, msarkis@wpi.edu

We consider a transmission problem where the interface does not align with the FEM triangulation. We consider a CutFEM method which is a discretization based on DG-Nistche techniques for unfitted meshes. In this talk we review the main mathematical tools to establish a priori error estimates and show how to use them to develop robust preconditioners. This is a joint work with Blanca A. de Dios, Kyle G. Dunn, and Simone Scacchi.

Positivity-preserving Limiters for the Piecewise-PN Equations

Minwoo Shin, Iowa State University, mws@iastate.edu

Transport problems are computationally expensive to numerically simulate because they require sufficient phase space resolution in order to accurately represent the exact kinetic distribution. A common approach is to use the PN equations, which are rotationally invariant and converge in L2 sense to the solution of transport equation as N tends to infinity. However, in the multidimensional setting, the PN equations often produce negative particle concentrations, which is physically incorrect. In the literature there exist many approaches to preserve positivity of the particle concentration. In our approach we introduce the piecewise-PN equations to solve the kinetic transport equation and develop for these equations a modified version of the Zhang-Shu positivity-preserving limiters to achieve physically meaningful positive particle concentrations.

A Multiscale Discontinuous Galerkin Method for 1D Stationary Schrodinger Equations

Wei Wang, Florida International University, weiwang1@fiu.edu

In this talk, we will introduce a multiscale discontinuous Galerkin method for one-dimensional stationary Schrodinger equations which have highly oscillating solutions. Because of the oscillatory behavior of the solutions, traditional numerical methods require extremely refined meshes to resolve the small scale structure of solutions, thus the computational cost is huge. The main ingredient of our method is to incorporate the small scales into finite element basis functions so that the method can capture the multiscale solution on coarse meshes. We prove that the DG approximation converges optimally with respect to the mesh size h in L2 norm without the constraint that h has to be smaller than the wave length.

Positivity-preserving Well-Balanced Discontinuous Galerkin Method for Tidal Bores

Yulong Xing, Ohio State University, xing.205@osu.edu

The positivity-preserving well-balanced discontinuous Galerkin method is employed to solve the shallow water equations on an unstructured triangular mesh and their applications in computational hydrology. The tidal bores in an idealized estuary problem are simulated to study the development and evolution of the tidal bores from different amplitudes of incoming tidal waves and topography of the river bed bottom. The numerical experiments demonstrate that the DG method can be applied successfully to this class of problems.

Direct Discontinuous Galerkin Methods for Keller-Segel Chemotaxis Equations

Jue Yan, Iowa State University, jyan@iastate.edu

We develop a new direct discontinuous Galerkin (DDG) methods to directly solve Keller-Segel Chemotaxis equations. Different to available DG methods or other numerical methods in literature, we introduce no extra variable to approximate the chemical density gradients but solve the system directly. With P^k polynomial approximations, we observe no order loss and optimal (k+1)th order convergence is obtained. The reason that DDG methods is convergent with optimal orders is that DDG methods have the super convergence property on its approximating to solution gradients. With Fourier (Von Neumann) analysis technique, we prove the DDG solution's spatial derivative is super convergent with at least (k+1)th order under moment norm. We show the cell density approximations are strictly positive with at least third order of accuracy. We also carry out second order finite difference schemes to simulate the liquid and semi-solid models of chemotaxis. The pattern formations observed are consistent to those in literature.

An EDG Method for Distributed Control of Convection Diffusion PDEs

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In this talk, we present a priori error analysis of an embedded discontinuous Galerkin (EDG) method for a distributed optimal control problem governed by convection diffusion PDEs. We derive an optimal priori error estimates for the state, adjoint state and the optimal control. 2D and 3D numerical experiments are provided to confirm our theoretical results.

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MS22 "Mathematically-based Insights into Health and Disease"

Cecilia Diniz Behn, Colorado School of Mines, cdinizbe@mines.edu
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Data Assimilation Approaches Using Self-monitoring Data to Forecast and Phenotype Type 2 Diabetes

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Type 2 diabetes affects 8% of the population and is a deadly and costly chronic disease. Despite these negative repercussions and the substantial efforts to mitigate the consequences of type 2 diabetes, treatment is not achieving its desired effectiveness because the disease is both complex to treat and poorly understood. Treatment, consisting of medication in combination with changes in diet and exercise, is a problem of self-management where quantifying the effects of choices is nonlinear, nonstationary, and personal. Here we will introduce how data assimilation can be used to help solve both the self-management problem, through personalized forecasting, and the biological problem, through phenotyping via parameter estimation. Moreover, data assimilation has three broad levers affecting its effectiveness, the model, the assimilation machinery, and the evaluation metric. We will discuss the effectiveness of glucose forecasting and parameter estimation for a variety of endocrine models, assimilation machinery (e.g., unscented Kalman filters, Markov Chain Monte Carlo methods, etc.), and evaluation metrics.

Comparison of Methods for Calculating the Rate of Appearance of Exogenous Glucose

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Insulin resistance (IR) is a crucial element of the pathology of metabolic syndrome, which now affects more than a third of the population in the United States. Understanding glucose dynamics following a meal is crucial for assessing IR under physiological conditions and identifying tissue specificity of IR. Using an oral glucose tolerance test (OGTT) protocol with two stable isotope tracers, both the rate of appearance of exogenous glucose (Ra_exo) and the suppression of endogenous glucose may be computed. In previous work, investigators have proposed several different methods for computing Ra_exo. The aim of this project was to compare these methods for calculating Ra_exo and to determine methodological effects on estimates of insulin sensitivity. Methods were applied to OGTT data from a group of obese adolescent girls and compared based on inter-method variability and known physiology. Estimates of Ra_exo were incorporated into differential equations-based models of whole body glucose-insulin dynamics, and method dependence of insulin sensitivity measures was assessed. Improved understanding of interactions between exogenous and endogenous glucose dynamics will facilitate the characterization of IR in individual patients and different disease conditions and may support the development of targeted therapeutic approaches.

Toward a Mathematical Model of Hemostasis

Nicholas Danes, Colorado School of Mines

Hemostasis is the process by which a blood clot forms to prevent bleeding. The formation time, size and structure of a clot depends on the local hemodynamics and the nature of the injury. Extravascular injuries, those which occur outside the vessel, have not been extensively modeled or understood. To understand such injuries, both experimental and computational models of hemostasis must be simultaneously developed from the ground up. Here we develop and validate a computational model against analogous experimental results for the fluid dynamics inside a microfluidic bleeding chip. Future steps to further communicate the experimental and computational models are also presented for modeling the transport and reactions of the platelet populations.

Analyzing the Role of Blood Flow in Glaucoma Using Mathematical Modeling
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Primary open angle glaucoma is the second-leading cause of blindness worldwide and is characterized by progressive retinal ganglion cell death and vision loss. Elevated intraocular pressure is the primary risk factor for glaucoma, but recent studies have shown that impaired blood flow and oxygen delivery are also significant factors contributing to retinal ganglion cell destruction. It is unknown, however, whether changes in blood flow to the retina are the cause or effect of retinal ganglion cell death, and a combined experimental and theoretical approach is needed to analyze the relationship between blood flow impairment and glaucoma. In this talk, recent data-driven theoretical models will be presented that predict how issues with blood flow regulation could lead to the impaired oxygenation seen in experimental glaucoma data. Then, an updated model of the retinal vasculature based on confocal microscopy images will be introduced. This model uses a Green's function method to predict oxygenation of the retina in a realistic vascular network, and preliminary results predict oxygen saturation in the retinal arteriolar and venular trees. The predictions from this mathematical model will be used to address the controversy of the cause-and-effect relationship between retinal ganglion cell death and impaired blood flow in glaucoma.

Fibrin-Thrombin Binding Under Flow
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Thrombin is an important enzyme for blood clot formation. One of its many roles is cleaving fibrinogen into fibrin, which polymerizes into a gel matrix and stabilizes a growing clot. Interestingly, after the fibrin matrix forms, thrombin continues to bind via two binding sites, one of high affinity and one of low affinity. It has been shown experimentally that once thrombin is incorporated into a preformed fibrin matrix, it stays bound for extended periods of time and is resistant to removal by flow and chemical inhibitors. It is not clear how thrombin stays bound for so long given the kinetic rates for thrombin binding found in the literature. Here we present a mathematical model that includes fibrin-thrombin binding, physical and spatial effects of fluid flow, and solute transport. Preliminary results suggest that there is a population of thrombin bound to the high affinity sites; the sustained thrombin measurements seen experimentally are likely due to a combination of spatial effects of the experiment itself and dynamic movement of thrombin between high and low affinity binding sites.

Interacting Bumps Model of Working Memory Limitations
Nikhil Krishnan, University of Colorado at Boulder, nikr9200@colorado.edu

Working memory allows animals to store information for limited periods of time. While working memory can store multiple items simultaneously, increasing the number of items decreases the accuracy of storage. We analyze the dynamics of a neural field model of working memory, which uses stimulus-tuned neurons connected by recurrent excitation and lateral inhibition. Connectivity is represented by the kernel of an integral term. Specifically, we study the dynamics corresponding to the retention of multiple visual angles presented simultaneously. Remembered locations are represented by localized regions of persistent activity, called bumps. We analyze their dynamics during the memory retention period by developing low-dimensional equations for the bump interfaces, the locations where their activity level equals the firing threshold of the neural field. With these effective equations, we can quantify how the relative placement of the visual stimuli impacts the dynamics of the remembered location. In particular, remembered angles can attract or repulse one another depending on their distance from one another. The impact of stochasticity is also considered; we show it causes bumps to wander, adding to the error that accumulates over time.

Towards Personalized Verification and Synthesis for the Artificial Pancreas
Taisa Kushner, University of Colorado at Boulder, taisa.kushner@colorado.edu

People with type-1 diabetes exhibit a large range of variations in the physiological characteristics that affect their response to blood glucose levels, including gender, weight, insulin sensitivity, dietary habits, exercise and hormonal fluctuations. At the same time, control algorithms for the artificial pancreas can be tuned using numerous parameters that affect the correctness and performance of the closed-loop system. We present a new approach using nondeterministic relational models of human insulin-glucose regulation inferred from patient data using multiple time scales. Treating the equations of this model as constraints, we model the behavior of the entire closed loop system over a time horizon using an optimization problem. Next, we demonstrate this approach using patient data gathered from a previously conducted outpatient clinical study and perform reachability analysis for a PID control scheme taken from the literature.

Network Science and the Ongoing Evolution of Malaria's Virulence in Humans and Apes
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Key to malaria's ongoing transmission is the fact that humans develop only a weak immunity. This is due to the parasite's evasion of the immune system by sequential expression of camouflage-like proteins on the surface of infected red blood cells. The genetic variation within the camouflage-encoding var genes is sufficiently high dimensional that immunity to a single camouflage variant doesn't prevent future infections, and even exposure to multiple variants provides only partial immunity. A complete analysis of var gene evolution has been blocked by two complicating factors. First, each parasite genome contains a unique set of ~60 different var genes. Second, this genetic repertoire rapidly recombines within human hosts. Together, these rule out the traditional phylogenetic toolkit. Here, we overcome these difficulties with a framework that maps rapidly recombining genes to networks in which evolutionary constraints are revealed in large-scale network structures. Applying this approach to multiple genomes, we identify rapidly evolving locations on the camouflage proteins, highlighting the mechanisms and constraints underlying the ongoing evolution of var genes. We then investigate an expanded dataset that includes var genes from ape-infecting malaria parasites, framing the epidemiological struggle against malaria in humans in a broader evolutionary context.

Approximate Bayesian Computation Methods for Parameter Estimation of SEIR Model
Kaitlyn Martinez, Colorado School of Mines, kmartinez@mines.edu

This project aims to extend the framework of stochastic analysis epidemic models that are derived from a set of ordinary differential equations (ODEs) and are based on the underlying biological and spatial spread of disease. By implementing Bayesian Inference, this project proposes novel parameterizations of infectious disease models in the susceptible, exposed, infectious, removed (SEIR) class, and explores various methods to estimate these parameters. Approximate Bayesian Computation (ABC) is used for estimating population distributions and the model parameters. ABC uses a batch of proposed parameters to generate simulated data that can be assess as close to or far from the real data under some norm. Historically, these methods are limited from extension to spatial models, as many SEIR models consider infectious counts, rather than proportions of people relative to the total population. Thus, there are considerable modeling challenges that must be assessed in conjunction with these computational difficulties to develop viable spatial models. The final stage of this project aims to develop ABC methods that can propose parameters and generate populations using proportions. This will allows us to extend the framework to stochastically analyze systems of PDEs, which is novel is the spatial epidemic literature.

Establishing a Theoretical Framework for Ultradian Forced Desynchrony Protocols
Nora Stack, Colorado School of Mines, nstack@mymail.mines.edu

In adult humans, the molecular circadian clock typically has an intrinsic period of just over 24 h. This clock entrains to the 24 h day by environmental factors such as light, eating, and exercise. To isolate circadian characteristics, the rest-activity cycle and the circadian cycle must be desynchronized. This desynchronization is achieved using forced desynchrony (FD) protocols in which the participant is exposed to a light/dark cycle with a period that is outside the range of entrainment of the circadian clock. Recently, researchers have developed resource-effective ultradian FD protocols with short light/dark cycles (e.g. 1-4 h). However, the effects of protocol design have yet to be formally studied, and it is cost prohibitive to optimize them experimentally. Using a mathematical model of the human circadian pacemaker, we have sought to optimize the implementation of ultradian FD protocols in the lab to accurately assess the intrinsic period of the circadian pacemaker. We assessed many different protocol parameters including light/dark duration, light levels, study length, and phase onset. This analysis can be used by researchers to inform protocol design for future ultradian FD protocols.

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MS23 “Advances In Higher-Order and Reduced-Order Numerical Methods"

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Efficient High-order Conservative Upwind Schemes for the Wave Equation on Overlapping Grids

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I will present an efficient, high-order, conservative upwind finite-difference scheme for the second-order wave equation in curvilinear geometries. Complex spatial geometry is discretized by use of overlapping component grids that interpolate solutions to one another. This grid interpolation may excite numerical instabilities in conventional nondissipative methods and it is common practice to add some artificial dissipation. The upwind flux incorporated via an exact d'Alembert solution provides a natural dissipation with no free tuning parameters that keeps the scheme stable on overlapping grids. I will give a formally exact conservative differential-difference equation from which successively high-order approximations may be extracted. These schemes are 'efficient' in the sense that if the overall scheme is viewed as a modification to the standard centered-difference approximations to the wave equation then the contribution to cost from the upwind dissipation is minuscule.

A Split-Step Finite-Element Method for Incompressible Navier-Stokes Equations with High-Order Accuracy up-to the Boundary

Longfei Li, University of Louisiana at Lafayette, longfei.li86@gmail.com

Motivated by extending our new Added-Mass Partitioned (AMP) scheme for the fluid-structure interaction problems to the FEM framework, we develop an efficient FEM algorithm to solve the incompressible Navier-Stokes (INS) equations. The efficiency of the algorithm is achieved by solving the INS equations in the velocity-pressure reformulation using a split-step method so that the momentum and pressure equations are updated separately at each time step. Solving the pressure separately enables the use of standard finite-elements (e.g. Lagrange finite-elements of equal order) for both velocity and pressure. With a special treatment for the pressure boundary conditions, the algorithm recovers the optimal order of accuracy for both velocity and pressure up-to the boundary.

Muntz Polynomials with Applications to Numerical Solutions for Differential Equations

Yingwei Wang, University of Wisconsin - Madison, wywshtj@gmail.com

In general, solutions to the Laplacian equation enjoy relatively high smoothness. However, they can exhibit singular behaviors at domain corners or points where boundary conditions change type. In this talk, I will focus on the mixed Dirichlet-Neumann boundary conditions for Laplacian equation, and discuss how singularities in this case adversely affect the accuracy and convergence of standard numerical methods. Then, starting from the celebrated Weierstrass theorem on polynomial approximation, I will describe the approximation theory related to the so called Muntz polynomials, which can be viewed as a generalization of usual polynomials. Additionally, I will illustrate the idea of Muntz-Galerkin methods, and show that how they can overcome the difficulties to achieving high order accuracy for the problems with singularities.

Improving Numerical Boundary Derivative Recovery for Elliptic PDEs

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Many engineering applications, such as fluid structure interaction, chemical reactor design, and structural mechanics require accurate calculation of boundary derivatives as part of a numerical simulation. The usual strategy for calculating boundary derivatives involves post-processing: that is, one recomputes, e.g., by least squares, a new solution near the boundary from known superconvergence points that has improved approximation properties and then differentiates. In this talk we will discuss some recent work towards improving boundary derivative recovery

by enriching the finite element space instead of standard postprocessing techniques: we provide both a new theoretical framework and results on complex 2D geometries to validate the new approach.

Data-driven Filtered Reduced Order Model

Xuping Xie, Oak Ridge National Lab, xupingxy@vt.edu

We propose a calibrated filtered reduced order model (CF-ROM) framework for the numerical simulation of general nonlinear PDEs that are amenable to reduced order modeling. The novel CF-ROM framework consists of two steps: (i) In the first step, we use explicit ROM spatial filtering of the nonlinear PDE to construct a filtered ROM. This filtered ROM is low-dimensional, but is not closed (because of the nonlinearity in the given PDE). (ii) In the second step, we use a calibration procedure to close the filtered ROM, i.e., to model the interaction between the resolved and unresolved modes. To this end, we use a linear or quadratic ansatz to model this interaction and close the filtered ROM. To find the new coefficients in the closed filtered ROM, we solve an optimization problem that minimizes the difference between the full order model data and our ansatz. Although we use a fluid dynamics setting to illustrate how to construct and use the CF-ROM framework, we emphasize that it is built on general ideas of spatial filtering and optimization and is independent of (restrictive) phenomenological arguments. Thus, the CF-ROM framework can be applied to a wide variety of PDEs.

HDG-POD Reduced Order Model of the Heat Equation

Yangwen Zhang, Missouri University of Science and Technology, ywzfg4@mst.edu

We propose a new hybrid discontinuous Galerkin (HDG) reduced order modeling technique based on proper orthogonal decomposition (POD). We provide estimates for the error between the HDG solution and the HDG-POD solution in an idealized case, and we show the error converges to zero as the number of POD modes increases. We present 2D and 3D numerical results to illustrate the convergence analysis.

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MS24 "Applications of Algebraic Topology"

Brittany Terese Fasy, Montana State University, brittany@cs.montana.edu
Lori Ziegelmeier, MaCalester College, lziegel1@macalester.edu

Persistence-Based Summaries for Metric Graphs

Ellen Gasparovich, Union College, gasparoe@union.edu

In this talk, we will focus on giving a qualitative description of information that one can capture from metric graphs using certain topological summaries. In particular, we will give a complete characterization of the persistence diagrams in dimension 1 for metric graphs under a particular intrinsic setting. We will also look at two persistence-based distances that one may define for metric graphs and discuss progress toward establishing their discriminative capacities. This is joint work with Maria Gommel, Emilie Purvine, Radmila Sazdanovic, Bei Wang, Yusu Wang, and Lori Ziegelmeier.

Node Filtrations in Biological Data

Chad Giusti, University of Delaware, cgiusti@udel.edu

Using persistent homology for data analysis relies on the existence of a natural filtration on a complex derived from the data of interest. In many common TDA complexes, like the Vietoris-Rips complex of a point cloud, the nodes are present throughout the filtration and the data is encoded in a weighting on the faces. Here, we study biological systems where the filtration naturally occurs on the level of nodes, with all other data prescribed by this filtration. Examples will include semantic learning and fungal growth.

Higher Structures in Topological Data

Ryan Grady, Montana State University, r.e.grady@gmail.com

I will outline some applications of higher structures/categories in topological data analysis. I will discuss how multidimensional problems are naturally organized by higher categories. More explicitly, I will discuss applications to higher Morse functions and multidimensional persistence.

Metric Thickenings of Euclidean Submanifolds

Joshua Mirth, Colorado State University, mirth@math.colostate.edu

Given a sample X from a manifold M embedded in Euclidean space, it is possible to recover the homotopy type of M by building a Vietoris-Rips simplicial complex, or a Cech simplicial complex, with vertex set X. However, these simplicial complexes need not inherit the metric structure of the manifold; a simplicial complex is metrizable if and only if it is locally finite. We define metric thickenings of X, called the Vietoris-Rips thickening and the Cech thickening, which are equipped with the 1-Wasserstein metric instead of the simplicial complex topology. We show that for Euclidean subsets M with positive reach, the metric thickenings satisfy metric analogues of Hausmann's theorem (the Vietoris-Rips thickening of M is homotopy equivalent to M for scale parameters less than the reach) and the nerve lemma. In contrast to Hausmann's original theorem, our homotopy equivalence is given by canonical maps in both directions, is realized by linear homotopies from the map compositions to the corresponding identity maps, and is furthermore a deformation retraction.

Applications of Persistence to Time Series Analysis

Elizabeth Munch, Michigan State University, muncheli@msu.edu

A time series is simply a stream of data. One way of studying this stream of data is through the Takens embedding, which puffs out the dynamics of the system into a geometric object which can be studied. In this talk, we will look at how methods from topological data analysis, such as persistent homology, can be combined with machine learning methods in order to quantify, classify, and predict behaviors from these data streams. We will discuss these methods in the context of two applications from different domains. First, we will discuss the phenomenon of chatter in machining dynamics. Chatter is the undesirable behavior exhibited by a cutting tool which is characterized by large amplitude vibrations that result in non-smooth metal parts, as well as an intense noise. Combining Taken's embedding theorem, persistence, and machine learning methods gives 97% accuracy when attempting to predict and prevent this behavior. Second, we will use persistence to quantify a diurnal cycle recently observed in IR hurricane data. In this case, we turn a matrix valued time series into a persistence diagram valued time series and investigate the resulting periodic behavior in persistence diagram space.

Topological Methods on Ion Bombardment Patterns
Rachel Neville, University of Arizona, rachel.neville629@gmail.com

When a nominally flat binary compound is bombarded with a broad ion beam, disordered hexagonal arrays of nanodots can form. In time, the pattern will either resolve to a perfect hexagonal array, or defects, which limit the utility of the nanodot array, " set in" or grow. Understanding the conditions lead to lasting defects can be challenging due in part to the complexity of patterns. However, model parameters are reflected directly in dynamic data in a way made accessible by studying topological structure. Persistent homology summarizes the topological structure of the evolving patterns and serves as a lower dimensional lens through which to investigate the influence of nonlinear parameters on pattern formation and defects.

Topological Features in Random Geometry
Chris Peterson, Colorado State University, peterson@math.colostate.edu

This talk will describe interactions between the fields of real algebraic geometry, probability theory, and algebraic topology. In particular, we consider special cases of the problem of determining the type and frequency of topological structures that arise as the real zero locus of a collection of random homogeneous polynomials.

Mathematical Morphology Applied To Non-Directed Simple Graphs
Catherine Potts, Montana State University, catherine.potts@montana.edu

In mathematical morphology, the skeleton of an object can be found by collecting the centers of maximal disks that are contained inside the object and share at least two points with the boundary of the object. Classical algorithms use sequences of operations from mathematical morphology such as dilation and erosion to determine the skeleton. We are working to apply the concept of a skeleton to non-directed simple graphs, built from sampling different geometric objects, to aid in identifying the underlying manifolds found in large data sets. Since the set of graph vertices does not have a natural complement and thus no immediate notion of boundary, our preliminary approach starts by defining an estimate of graph boundary built from growing shells of fixed radius around each vertex in the graph and subsequent thresholding of the distribution of the number of vertices per such shell. Once the boundary has been determined, the skeleton can be found using an adaptation of the dilation, erosion, and opening methods known from mathematical morphology, acting on the nearest neighbors of the boundary set. Promising results from data sets sampled from geometric objects, trees, and a Sierpinski carpet will be presented.

Dualities and Combinatorics of Simplicial Sheaves of Vector Spaces on Finite Topologies
Emilie Purvine, Pacific Northwest National Laboratory, emilie.purvine@pnnl.gov

Sheaf theory provides a compelling and canonical model for data integration problems by allowing data to sit on top of a topological space that models the interaction of data sources. However, as this is a "modeling framework" there are choices that must be made in the problem set up that may affect the final results. In recent work we have explored the combinatorial space of these choices to understand how much of an effect they may have. We have discovered that there are a number of dualities that arise which collapse some of the choices into a single model. Further modeling questions about the choice of stalks and restriction functions do not provide dualities, but instead may force the choice of other stalks or restrictions. Additional questions like whether inferences are being made about global information from local, versus the converse, introduce other dualities in sheaf construction, in particular in the functor used to satisfy the gluing axioms. In this talk I will motivate our study, provide the analysis of the combinatorics of dualities of sheaves over finite topologies, and provide some advice to a potential modeler attempting to set up such a framework.

Optimally Topologically Transitive Orbits in Two-dimensional Discrete Dynamical Systems
Patrick Shipman, Colorado State University, shipman@math.colostate.edu

Every orbit of a rigid rotation of a circle by a fixed irrational angle is dense. However, the apparent uniformity of the distribution of iterates after a finite number of iterations appears strikingly different for various choices of a rotation angle. Motivated by this observation, we introduce a scalar function on the orbits of a discrete dynamical system defined on a bounded metric space, called the linear limit density, which we interpret as a measure of an orbit approach to density. Any discrete dynamical system defined by an orientation-preserving diffeomorphism of the circle has an orbit with a larger linear limit density than any orbit of the rigid rotation by the golden number. We determine linear limit densities of orbits of two-dimensional discrete dynamical systems and random walks.

Applications of Multidimensional Persistence
Matthew Wright, St. Olaf College, wright5@stolaf.edu

Multidimensional persistent homology is highly relevant in the analysis of noisy data, as it offers the ability to filter by two or more parameters simultaneously. However, the algebraic complexity of multidimensional persistence modules makes it difficult to extract useful invariants in this setting, and until recently there was no available software for using multidimensional persistence in practice. In this talk I will summarize the RIVET software project, which aims to enable the use of two-dimensional persistence in real-world applications. I will highlight current work with students at St. Olaf College to apply RIVET real data, particularly data arising from Wikipedia, networks, and the natural sciences. I will demonstrate ways in which 2-D persistence can identify topological and geometric structure in complex, high-dimensional, multi-parameter data.

The Topology of Biological Aggregations: Experiments and Simulations
Lori Ziegelmeier, Macalester College, lziegel1@macalester.edu

We apply tools from topological data analysis to experimental and simulation data of models inspired by biological aggregations such as bird flocks, fish schools, and insect swarms. Our data consist of numerical simulation output from the models of Vicsek and D'Orsogna as well as experimental data of pea aphids and associated models. These models are dynamical systems describing the movement of agents who interact via alignment, attraction, and/or repulsion. Each simulation time frame is a point cloud in position-velocity space. We analyze the topological structure of these point clouds. To interpret the persistent homology of our results, we introduce a visualization that displays Betti numbers over simulation time and topological persistence scale. We compare our topological results to order parameters typically used to quantify the global behavior of aggregations, such as polarization and angular momentum. The topological calculations reveal events and structure not captured by the order parameters.

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MS25 "Ecology and Evolution of Infectious Diseases"

Majid Bani-Yaghoub, University of Missouri Kansas City, baniyaghoubm@umkc.edu

Transmission Dynamics of Emerging and Zoonotic Infectious Diseases Governed by the Triad of Ecology, Evolution and Anthropogenic

Majid Bani-Yaghoub, University of Missouri - Kansas City, baniyaghoubm@umkc.edu

Zoonotic diseases are caused by infections that are shared between animals and humans. Emerging infectious diseases are infections with increasing occurrences. In recent years, special attention has been given to emerging and zoonotic infectious diseases with respect to interactions between ecology, evolution and anthropogenic activities. Several studies indicate that developing resistance to antibiotics and disinfectants allows various pathogens to survive within host tissue and environment, respectively. Nevertheless, the influence of other evolutionary responses (e.g. host exploitation or increased pathogen shedding) on transmission dynamics of emerging and zoonotic infectious diseases has been less studied. In the present work, we compare the feasibility of above-mentioned evolutionary responses via analysis and simulation of a multi-strain Susceptible-Infected-Susceptible model with intermittent shedding and free-living pathogen. Using the example of Escherichia coli O157:H7, it is shown that drug resistance favors coexistence of strains, whereas host exploitation leans towards single strain infection. Developing resistance to disinfectants can be the most detrimental evolutionary response, where the entire stability region of endemic equilibria is divided between coexistence and single infection. In addition, we show that the effectiveness of control and preventive policies is assessed more accurately when interactions between ecology, evolution and anthropogenic activities are taken into account.

Origins and Patterns of Foodborne Bacterial Resistance: Implication for Antimicrobial Comparison Based on MIC Frequency Distribution

Majid Jaberi-Douraki, Kansas State University, jaberi@k-state.edu

Minimum Inhibitory Concentration (MIC) is defined as the susceptibility of foodborne pathogenic and commensal bacteria, such as Escherichia coli, Enterococcus spp., and Salmonella spp., to an antimicrobial agent based on the minimum concentration inhibiting their visible growth. Antimicrobial susceptibilities vary over time and by hosts, creating complex patterns which requires us to study and unravel drug resistance behavior and missing similarity links. The National Antimicrobial Resistance Monitoring system in the U.S. (NARMS) provides yearly reports on foodborne bacteria resistance including 54 different antimicrobials which fall under the purview of this study. Using the NARMS data from 1996 to 2013 and novel comparison-based algorithms, we identified several different antimicrobial agents in four hosts that exhibited analogous resistance profiles within this timeframe. Our results show that kanamycin antimicrobial susceptibilities display similarities in their behavior with amikacin and ceftiofur in Salmonella spp. from cattle isolates at retail sampling points. Amoxicillin-Clavulanic acid also expressed temporal correlation with Streptomycin, ceftriaxone, and kanamycin in E. coli from chicken isolates at slaughter sampling points. Based on our findings, we discovered relations between drugs that could further improve prediction and categorization of bacterial resistance to existing and modern antimicrobials beyond their clinical composition (classification).

Information Loss for Describing Antimicrobial Resistance Dynamics in Populations due to Breakpoint-based Categorization

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Isolate susceptibility to an antimicrobial is measured as the lowest drug concentration inhibiting growth of the isolate, termed the minimum inhibitory concentration (MIC). An isolate is conventionally categorized as Susceptible, Intermediate, or Resistant. MIC frequencies for pathogens in a host population are reduced into dichotomous (Susceptible, Resistant) or categorical (Susceptible, Intermediate, Resistant) variables. Such data categorizations are known to cause losses of information and reduces analytical power and flexibility compared to analyzing underlying frequency distributions. The U.S. National Antimicrobial Resistance Monitoring System (NARMS) monitors resistance in foodborne bacteria at food animal processing and retail product points. For the

NARMS 1996Γ2013 datasets, we discovered significant changes in MIC frequency distributions between consecutive years, where categorization-based analyses concluded no change. Considering 54 antimicrobial drugs, we found that 50% of year-to-year comparisons contained significant changes that were missed by conventional categorization. Similarly, in 71% of the antimicrobials, bacterial species, and host combinations, MIC frequency distributions differed significantly between animal processing and retail product sampling points, while categorization-based analyses detected no difference. Our findings show that analyses using the breakpoint-based categorizations of the MIC data miss significant developments in the resistance distributions between the sampling points or time periods.

Parasite Species Interactions and Epidemics
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Most hosts support multiple species of parasites, yet few parasites have epidemics. Whether a parasite has epidemics can be determined by other parasite species. In foliar fungal parasites infecting the widespread grass tall fescue, epidemics of Rhizoctonia solani can be reduced by a second parasite, Colletotrichum cereale. Unlike Colletotrichum, Rhizoctonia is transmitted not only host-to-host but also soil-to-host (environmental transmission), and Rhizoctonia induces greater host mortality. To understand the conditions allowing epidemics of Rhizoctonia, we analyzed a model with two parasites where one parasite can infect leaves already infected by the other. This model is identical in form to models of intraguild predation among competitors with an explicit resource (susceptible hosts). The model allows for a continuum of transmission for the intraguild parasite from pure environmental transmission to pure host-host transmission. If there is no environmental transmission, alternative stable states, with two stable single-species equilibria, are possible when the intraguild parasite is a poorer competitor. If there is any environmental transmission, the rate of environmental transmission determines whether there is stable coexistence or whether the intraguild parasite excludes its competitor, consistent with data. These results help to define the conditions under which one parasite can prevent epidemics of another parasite.

Understanding Variance Reduction Behavior in Diversity-disease Studies
Peter Shaffery, University of Colorado at Boulder, pesh5067@colorado.edu

The commonly observed negative correlation between species richness and pathogen prevalence, typically referred to as "the dilution effect", has received a substantial amount of theoretical and experimental attention over the past decade. Less attention has been paid, however, to the decrease in variability of pathogen prevalence across study units and species richness, the so-called "variance reduction effect". We analyze a simple model of a randomly assembled community undergoing an SIR epidemic to place upper bounds on the variance of the community R_0, and in doing so determine the community-level factors which control the strength and direction of the variance changes. We furthermore analyze how a changing variance may obscure the true role of biodiversity in disease risk, particularly in the case where disease prevalence depends non-monotonically on species richness.

Deciphering Prevalence and Dynamics of Collateral Antimicrobial Resistance within and among Bacterial Species
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Antimicrobial drug application to treat bacterial infections leads to dissemination of bacterial antimicrobial resistance (AMR) to the treatment and other antimicrobials causing collateral AMR. Deciphering prevalence and dynamics of the collateral AMR patterns is challenging, but necessary for informing the development and evaluation of public health strategies to curtail AMR. Multiple-drug resistant Markov networks (MDR networks) have been used to describe the collateral AMR ΓÇô co-occurrence of phenotypic AMR to various drugs in a bacterial species. Commensal bacteria can act as reservoirs of AMR genes for pathogens, necessitating to control collateral AMR spread in commensal and pathogenic bacteria which inhabit the same ecological niches. We investigated the prevalence and dynamics of the patterns of joint AMR distributions in a commensal (Escherichia coli) and a pathogenic (Salmonella enterica) bacteria isolated from the same food-animals or food products at retail, using the National Antimicrobial Resistance Monitoring System data from 2004 to 2012. Based on our findings, we observe a temporal nature of the MDR networks, suggesting complex trends of the between-species spread of collateral AMR.

Studying the temporal joint AMR distributions for multiple bacteria in same hosts can facilitate detection of multi-drug AMR and identification of its origins among commensal or pathogenic bacteria.

Network Spread of Invasive Species and Infectious Diseases
Patrick Shipman, Colorado State University, shipman@math.colostate.edu

Long-distance transportation connections and landscape heterogeneity can be factors in the spread of an infectious disease or an invasive species. We introduce a mathematical model that combines a vector-based transportation network with models for continuous spread and apply the model to the invasion of cheatgrass in Rocky Mountain National Park.

Bayesian Inference in Within-Host Disease Models
Sama Shrestha, University of Colorado at Boulder, sama.shrestha@colorado.edu

An important aspect of epizootic disease transmission modeling is to infer the extent to which small-scale processes affect large-scale dynamics. Hence, understanding the dynamics behind how a viral infection spreads through an individual can prove useful in modeling the spread of the disease throughout the community. In our experimental system, insect herbivores become infected with baculovirus after consuming infected soybean leaf tissues. We have previously shown that the mortality rate of these insects is governed by their feeding preferences which motivates our within-host model. Through time series data collected on the number of virion cells inside the insect host, we perform inference on the parameters governing the host-virus growth dynamics. Our within-host model is a set of ordinary differential equations based on the predator-prey interaction model. We use Markov Chain Monte Carlo algorithms to make inference about the parameters and to quantify the uncertainty that arises in our dynamical system.

Optimal Control Strategy for Abnormal Innate Immune Response
Jinying Tan, Huazhong Agricultural University, jytan@mail.hzau.edu.cn

Optimal control strategy for abnormal innate immune response Abstract: In this talk, we discuss how to adopt optimal control strategy to obtain a good therapeutic effect when innate immune system failure in protecting us from the infection of the virus. The model established by the optimal control theory not only can be used to predict the behavior of the system, but also can help us to find a proper method to intervene and control the behaviors of the system.

Modeling Environmentally Transmitted Diseases
Jin Wang, University of Tennessee at Chattanooga, jin-wang02@utc.edu

We present a few examples in mathematical modeling of environmentally transmitted diseases, including cholera, foot-and-mouth disease, and brucellosis. An emphasis of these studies is the interplay of various ecological, biological, and environmental factors that shape the complex pattern of disease dynamics. In particular, we examine the impact of seasonal fluctuation on the evolution and transmission of such diseases. Models based on differential equations will be presented, and both analytical and numerical results will be discussed.

Mathematical Modeling of Cholera Epidemics
Xueying.Wang, Washington State University, xueying@math.wsu.edu

Cholera is a severe water-borne disease caused by the bacterium Vibrio cholerae. In this talk, I will present some recent investigations of cholera epidemics through mathematical modeling and analysis by using ODE and PDE models.

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Poster Presentation

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Filtered Discrete Ordinate Equations

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We develop a filtered modification of the radiation transport equation discretized over discrete ordinates (S_N). We will analyze certain choices of quadrature sets and under what conditions do our approximations converge to the true solution, and what is the order of the convergence. We will look at how the convergence depends on the smoothness of the solution, and how the filter affects the smoothness of certain interpolations of the numerical solution. We present numerical results to certain classical problems to demonstrate the effectiveness of the method.

Graph-Based Geometrical Data Analysis

Carrington Metts, College of William and Mary/ Montana State University, cametts@email.wm.edu

We are interested in geometrical data analysis based on graphical representations. One inherent characteristic of a graph is its dimension. While various definitions of graph dimension have been proposed and used, we consider the dimension to be the characteristic exponent relating ball radius and volume (cluster aggregation dimension). Previous authors have averaged this dimension estimate over all scales and ball centers to get a single value for each graph. However, we observe that the above definition of dimension fails to consider the underlying shape of the graph. Instead, we define local dimension to be a scale-dependent graph property that relates ball radius and shell volume. Additionally, based on this method of scale-dependent dimension, we have investigated the concept of a boundary for graphs. Specifically, we have developed a method to computationally determine the boundary of a graph without knowledge of an underlying manifold. Using these methods, we have successfully determined local dimension and boundary for a wide variety of epsilon-nearest-neighbor graphs, Cartesian graphs, trees, and fractals.

Tipping Times for Periodically Forced Stochastic Differential Equations with Piecewise Linear Drift

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Motivated by recent models of energy flux for the dynamics of Arctic sea ice, this project explores tipping times for periodically forced piecewise linear systems perturbed by weak additive white noise. The goal of this study is to determine the probability and expected time of a tipping event between two metastable states as a function of the parameters in the problem. Using analytical tools such as bifurcation theory, pathwise analysis of the underlying SDE, and the theory of large deviations, we explore how the deterministic and stochastic quantities in the problem govern the underlying statistics of the tipping time. Our results are further compared with Monte-Carlo simulations and numerical simulations of the Fokker-Plank equation.

Stochastic System Study of Urban Response and Recovery in the Aftermath of a Disaster

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