AN17-CT17-GD17 Abstracts

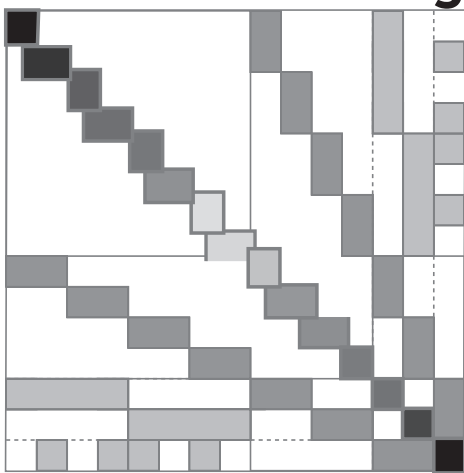## Annual Meeting

2017 SIAM

Figure courtesy Yuanzhe Xi, Ruipeng Li and Yousef Saad

July 10-14, 2017
David Lawrence Convention Center
Pittsburgh, Pennsylvania, USA

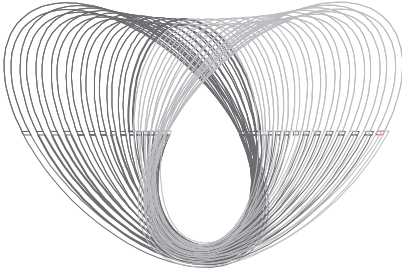**SIAM Conference on**

Figure courtesy Fabio Fagnani.

CONTROL & Its APPLICATIONS

July 10-12, 2017
David Lawrence Convention Center (DLCC)
Pittsburgh, Pennsylvania, USA

SIAM Conference on Industrial and Applied Geometry

July 10-12, 2017
David Lawrence Convention Center (DLCC)
Pittsburgh, Pennsylvania, USA

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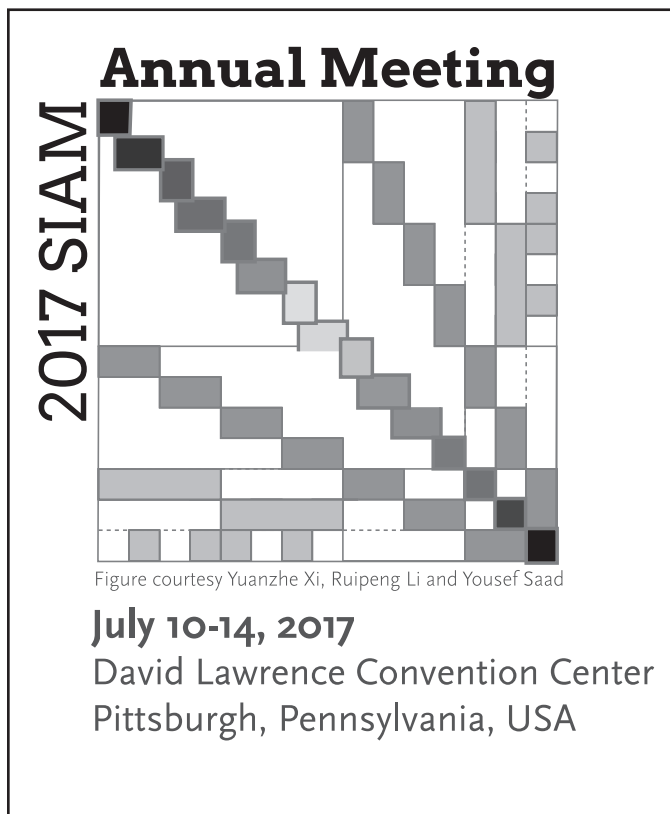Since 2008, SIAM has recorded many Invited Lectures, Prize Lectures, and selected Minisymposia from various conferences.
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AN17 Abstracts

2017 SIAM

Annual Meeting

Figure courtesy Yuanzhe Xi, Ruipeng Li and Yousef Saad

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IP1
Genetic Consequences of Range Expansion Under Climate Change

Range expansion is a crucial population response to climate change. Genetic consequences are coupled to ecological dynamics that, in turn, are driven by shifting climate conditions. We model a population with a reactiondiffusion system, coupled to a heterogeneous environment that shifts with time due to climate change. We decompose the resulting traveling wave solution into neutral genetic components to analyze the spatio-temporal dynamics of its genetic structure. Our analysis shows that range expansion under slow climate change preserves genetic diversity. However, diversity is diminished when climate change occurs too quickly. We show that populations with intermediate dispersal ability are best for maintaining genetic diversity. Our study also provides new insight regarding traveling wave solutions in heterogeneous environments. This is joint with Jimmy Garnier (CNRS).

Mark Lewis
University of Alberta, Canada
mlewis@math.ualberta.ca

IP2
Pattern Formation in the Drylands: Self Organization in Semi-Arid Ecosystems

Much of our understanding of spontaneous pattern formation was developed in the wetlands" of fluid mechanics. That setting came with fundamental equations, and benefitted from a back-and-forth between theory and experiment. Those investigations identified robust mechanisms for pattern formation, inspiring the development of equivariant bifurcation theory. Recently, these perspectives have been applied to dryland ecosystems, where aerial photographs reveal strikingly regular spatial vegetation patterns on large scales. In this far-from-pristine setting, there are no fundamental equations and no controlled laboratory experiments. Does the morphology of these patterns, readily monitored by satellite, convey information about the vulnerability of these ecosystems? We explore this within the setting of equivariant bifurcation theory, and via satellite image data.

Mary Silber
University of Chicago
Dept. of Engineering Sciences and Applied Mathematics
msilber@galton.uchicago.edu

IP3
Predicting Travel Time on Road Networks

Prediction of travel time on a road network has become commonplace and central to route planning. For example, commercial mapping services provide fastest routes and associated travel times, while emergency vehicle fleets use travel time predictions to better service metropolitan areas through strategic placement of parked vehicles. However, few systems in production provide information about the reliability of the predictions. Such information could be used for risk-averse routing in mapping services, and has the potential to improve ambulance positioning decisions, not only decreasing arrival and transport times, but also significantly impacting patient survival rates. I will describe approaches for probabilistic prediction of travel time on large-scale road networks. Estimates are based on location data from vehicles traveling along the road network;

for mapping services this is obtained from mobile phones, while for ambulance fleets it is obtained from automatic vehicle location devices. We demonstrate greatly improved accuracy relative to a system used in Bing Maps, and show the impact of our methods for improving ambulance fleet management decisions.

Dawn Woodard
Uber, USA
dawn@uber.com

IP4
Chaos and Learning in Spiking Neural Networks

Neurons in the brain must perform various computations including initiating motor commands, retaining memories, and generating complex spatiotemporal firing patterns over long time scales. It is able to accomplish these tasks in the presence of short time constants and seemingly random connectivity. Here I will describe some of our recent work regarding the dynamics of spiking neurons with random and specified time dependent synaptic connections. Under different parametric conditions, the network can exhibit states of regular firing, quasi-periodic firing, chaotic firing where the average rate is approximately constant, and chaotic firing where the rate and spike times are both chaotic. I will also show how a learning rule can be implemented to stabilize chaotic trajectories and also be used to train the neurons within network to directly follow a wide range of arbitrary spatiotemporal firing patterns, including actual neural firing data or even musical pieces.

Carson C. Chow
Laboratory of Biological Modeling
NIDDK, NIH
carsonc@niddk.nih.gov

IP5
Laplacian Matrices of Graphs: Algorithms and Applications

The Laplacian matrices of graphs arise in fields including Machine Learning, Computer Vision, Optimization, Computational Science, and of course Network Analysis. We will explain what these matrices are and why they arise in so many applications. In particular, we will show how Laplacian system solvers can be used to quickly solve linear programs arising from natural graph problems. We then will survey recent progress on the design of algorithms that allow us to solve these systems of linear equations in nearly linear time. We will focus on the role of graph sparsification and the recent discovery that it can be used to accelerate Gaussian elimination.

Daniel Spielman
Yale University
spielman@cs.yale.edu

SP1
AWM-SIAM Sonia Kovalevsky Lecture: Mitigating Uncertainty in Inverse Wave Scattering

Inverse wave scattering is an inverse problem for the wave equation, driven by a broad spectrum of applications. It is an interdisciplinary area that involves mathematical analysis, computational modeling, statistics and signal processing. This lecture will discuss one important challenge due the uncertainty of the model for inversion. Uncertainty is unavoidable in applications, not only because of noise, but

because of lack of detailed knowledge of complex media through which the waves propagate.

Liliana Borcea
University of Michigan
borcea@umich.edu

SP2

The John von Neumann Lecture: Singular Perturbations in Noisy Dynamical Systems

Consider a deterministic dynamical system in a domain containing a stable equilibrium, e.g., a particle in a potential well. The particle, independent of initial conditions eventually reaches the bottom of the well. If however, a particle is subjected to white noise, due, e.g., to collisions with a population of smaller, lighter particles comprising the medium through which the Brownian particle travels, a dramatic difference in the behavior of the Brownian particle occurs. The particle can exit the well. The natural questions then are: how long will it take for it to exit and from where on the boundary of the domain of attraction of the equilibrium will it exit. We compute the mean first passage time to the boundary and the probability distribution of boundary points being exit points. When the noise is small each quantity satisfies a singularly perturbed deterministic boundary value problem. We treat the problem by the method of matched asymptotic expansions (MAE) and generalizations thereof. MAE has been used successfully to solve problems in many applications. However, there exist problems for which MAE does not suffice. Among these are problems exhibiting boundary layer resonance, which led some to conclude that this was "the failure of MAE". We present a physical argument and four mathematical arguments to modify MAE to make it successful. Finally, we discuss applications of the theory.

Bernard Matkowsky
Northwestern Universtiy, USA
b-matkowsky@northwestern.edu

SP3

Past President's Address: The Future of SIAM: Looking to the Mathematicians of Tomorrow

During my tenure as SIAM president, I sought to emphasize that the S in SIAM stands for students by focusing on boosting our global presence and cultivating the next generation of mathematicians. To all the long-time SIAM members, can you guess how many new international chapters weve added since 2012? To all the new SIAM student members weve welcomed in that period, can you name all the ways SIAM can help you grow your careers? At the 2017 SIAM Annual Meeting I will invite our Student Chapters to use their own words to answer these important questions through a series of videos spanning several continents. The advances weve made should make us all proud. Of course, theres always more that SIAM can do as it continues to push ahead in order to remain at the vanguard of the scientific community.

Irene Fonseca
Carnegie Mellon University
Center for Nonlinear Analysis
fonseca@andrew.cmu.edu

SP4

James H. Wilkinson Numerical Analysis and Sci-entific Computing Prize Lecture: Tensors in Computational Mathematics

We show that in many instances, one would find a higher-order tensor, usually of order three, at the core of an important problem in computational mathematics. The resolution of the problem depends crucially on determining certain properties of its corresponding tensor. We will draw examples from (i) numerical linear algebra: fastest/stablest algorithms for matrix product, matrix inversion, or structured matrix computations; (ii) numerical optimization: SDP-relaxations of NP-hard problems, self-concordance, higher-order KKT conditions; and, if time permits, (iii) numerical PDEs: tensor network ranks. This talk is based on joint works with Ke Ye, with Shenglong Hu, and with Shmuel Friedland.

Lek-Heng Lim
University of Chicago
lekheng@galton.uchicago.edu

SP5

I.E. Block Community Lecture: From Flatland to Our Land: A Mathematicians Journey through Our Changing Planet

Mathematics is central to our understanding of the world around us. We live in a vast dynamical system, the many dimensions of which can be interrogated with mathematical tools. In this talk I will consider our changing climate. I will describe the scientific evidence that tells us how and why our climate is changing, and what the future may hold. In this journey I will pause at various waypoints to describe in more detail some of the insight different branches of mathematics are providing. Diverse examples will include applying ideas from dynamical systems research to create novel strategies for measuring the ocean mixing processes that are critical to the flow of heat and carbon through the Earth system, through to employing statistical learning techniques to improve future predictions of Arctic sea ice, currently in perilous decline. Climate change is one of the greatest challenges facing humanity. Responding to the challenge requires robust scientific evidence to inform policies. Opportunities for mathematicians to contribute to this important issue abound.

Emily Shuckburgh
British Antarctic Survey, United Kingdom
emily.shuckburgh@bas.ac.uk

SP6

W. T. and Idalia Reid Prize in Mathematics Lecture: Feedback Stabilization of Control Systems

A control system is a dynamical system on which one can act by using controls. For these systems a fundamental problem is the stabilization issue: Is it possible to stabilize a given unstable equilibrium by using suitable feedback laws? (Think to the classical experiment of an upturned broomstick on the end of one's finger.) On this problem, we present some pioneer devices and works (Ctesibius, Watt, Maxwell, Lyapunov...) and some more recent results on the finite-time stabilization and on the stabilization by means of time-varying feedback laws.

Jean-Michel Coron
Université Pierre et Marie Curie, France

coron@ann.jussieu.fr

JP1
Bio-Inspired Dynamics for Multi-Agent Decision-Making

I will present a generalizable framework that uses the singularity theory approach to bifurcation problems, and other tools of nonlinear dynamics, to translate some of the remarkable features of collective animal behavior to an abstract agent-based model. With the abstract model, analysis and design of decision-making between alternatives can be systematically pursued for natural or engineered multi-agent systems. To illustrate, I will apply the framework to explore and extend value-sensitive decision-making dynamics that explain the adaptive and robust behavior of house-hunting honeybees.

Naomi E. Leonard
Princeton University
naomi@princeton.edu

CP1
Modeling of Retinal Hemodynamics Coupled with Lamina Cribrosa Deformation

Retinal hemodynamics plays a crucial role in several ocular diseases. Clinical observations show significant correlations between hemodynamic alterations and vision impairment. However, the mechanisms giving rise to these correlations are not yet fully understood. We present a multi-scale mathematical model that combines the deformation of the lamina cribrosa in the optic nerve head with blood flow in the retina via a fluid-structure interaction problem. The lamina is modeled as a nonlinear, homogeneous, isotropic, elastic circular plate of finite thickness, which deforms under the combined action of intraocular pressure (IOP), cerebrospinal fluid pressure (CSFp) and scleral tension. The blood flow in the central retinal vessels is modeled as Stokes flow, where an incompressible Newtonian fluid fills a linearly elastic cylindrical shell. The walls of the central retinal vessels deform under an external pressure that varies along the vessel length to include CSFp, IOP and the effect of lamina cribrosa deformation. Intraocular retinal vessels are modeled as a network of resistances. Model results are compared to clinical data to estimate and quantify the mechanical factors that contribute to the influence of IOP and CSFp on retinal hemodynamics. The model suggests that changes in IOP have a stronger effect on retinal hemodynamics than changes in CSFp, and that this may be due to the fact that, unlike CSFp, IOP acts directly on the intraocular retinal vessels.

Lucia Carichino
Worcester Polytechnic Institute
lcarichino@wpi.edu

Giovanna Guidoboni
Indiana University Purdue University Indianapolis
gguidobo@iupui.edu

Alon Harris
Indiana University School of Medicine
alharris@indiana.edu

CP1
A Mathematical Model for Nutrient Metabolic

Chemistry

A model is presented for the rate of utilization and storage of carbohydrates, fats and proteins, is based on the chemical kinetics converting glucose and fatty acids to pyruvate and acetylCoA, which then enter the Krebs cycle to be converted to energy. The molecules can also be stored, with glucose converted to glycogen, fatty acids converted to fat, and amino acids converted to protein. The model consists of differential equations for the temporal changes of amino acids, proteins, glucose, glycogen, fatty acids, pyruvate and acetyl CoA in the body inside the gastrointestinal-blood barrier. The conversion rates are modeled as Hill's reactions, representing the fact that the reactions all involve enzyme kinetics. We assume that the rates at which the energy molecules enter the Krebs cycle are strictly controlled, resulting in the separation of glucose and fatty acids into subsystems where supply and usage compete with storage. We analyze short term dynamics with feeding and usage under conditions of balance and unbalance, and continuous (constant) and concentrated. Also, the model for long term dynamics shows that the the steady state of the fatty acid subsystem is unstable. Both the short term and long term models indicate that starting above the steady state leads to growth of the stored species. An analysis of a model for enzyme dynamics indicates that the steady-state level of an enzyme can depend on the rate of supply of the substrate.

Donald A. Drew
Rensselaer Polytech Institute
Dept of Mathematical Sciences
drewd3@rpi.edu

CP1
Influence of Autosomal Monoallelic Expression on Signal Transduction Through Network Motifs

In mammals, various genetic and epigenetic processes control relative expression of two alleles (copies) of a gene. Separate regulation of each allele is responsible for controlling the expression levels of the gene products. This phenomenon, called as clonal monoallelic expression or clonal MAE, leads to a random combination of genotypic states in a polyclonal population. A given cell in a polyclonal population may show following spectrum of states for a given genetic locus, beginning from unbiased to partially biased to mono-allelic. Increasing evidence shows that MAE can influence protein function for key proteins in disorders like schizophrenia, Alzheimers disease and cancer. Currently, it is not known under what conditions clonal MAE can impact the signaling behavior of cells. Here, we undertook a theoretical study on the influence of allelic bias on signal propagation through network motifs. Using detailed chemical kinetic models of network motifs typically found in large-scale signaling networks, we analyzed the influence of MAE on dynamic signal processing properties. Our initial results on a simple linear signaling cascade indicate that MAE at the receptor level controls the amplitude of the terminal signal while MAE at intermediate proteins of the motif control time dependent features like response time and signal duration but not the amplitude. This could probably explain all or none responses in many systems where MAE was detected at the receptor level.

Shibin Mathew
Department of Cancer Biology, Dana Farber Cancer Institute
Department of Genetics, Harvard Medical School
shibin_mathew@dfci.harvard.edu

Alexander Gimelbrant
Dana-Farber Cancer Institute
alexander_gimelbrant@dfci.harvard.edu

Suzanne Gaudet
Department of Cancer Biology, Dana Farber Cancer Institute
Department of Genetics, Harvard Medical School
suzanne_gaudet@dfci.harvard.edu

CP1
Reconstruction of Dynamical Trajectories of Cells Based on Single-Cell Data

The unprecedented accumulation of high-throughput single-cell data provides an essential opportunity for researchers to study the dynamics of biological systems. At the same time, it raises new questions and grand challenges in view of the key characteristics of these data that include high-dimensionality, multi-scale and randomness. In response, we develop a data-driven computational framework to map and reconstruct of dynamical trajectories of cells based on the high-dimensional molecular profiles from cross-sectional single-cell data. By integrating tools from dynamical systems, topology, geometry, statistics and machine learning, we first perform nonlinear dimension reduction on the data and then reconstruct the dynamic trajectories by fitting and testing on the tree structures. We apply this method in the analysis of cell developmental processes and provide novel insights into the field of mathematical and computational biology.

Lin Wan
Academy of Mathematics and Systems Science
Chinese Academy of Sciences
lwan@amss.ac.cn

CP1
Hydrodynamic Model for Pattern Formation in Tissues

In skin or intestinal epithelium, stem cells lie in periodic local areas. In those areas, whereas stem cells divide and differentiated without migration, the differentiated cells migrate out of the local areas actively, leading to mechanical stress gradients in the tissue. Not only the oriented migration of differentiated cells, but also the cell division and apoptosis introduce active stresses in the tissue. The Energy consumed in those active processes come from the ATP hydrolysis. Anisotopy of migration of differentiated cells might be caused by the internal signal pathways, or the density gradients of stem cells and differentiated cells in the tissues. We present one systematical hydrodynamic model to study the interplay of the mechanical stresses from those active processes and cell flow profiles in the tissue. Our mathematical framework considers the tissue as a viscoelastic fluid, with duplication, loss of the components and active particless migration driven by ATP hydrolysis. Linear stability analysis is conducted to reveal the long-wave instability inherent in the neighborhood of the constant steady states, including both spontaneous steady states and nonspontaneous steady states. The spatial patterns due to instability are observed in numerical experiments. Especially, new spatial patterns with spontaneous polarity are observed. Comparison with previous models will be presented in this talk.

Xueping Zhao
University of South Carolina
zhaoxueping0802@gmail.com

Qi Wang
University of South Carolina
Beijing Computational Science Research Center
qwang@math.sc.edu

CP2
Unsteady Flow of Thixotropic Fluid in a Slowly Varying Pipe

We use lubrication theory to develop the governing equations for unsteady axisymmetric flow of thixotropic fluid along a slowly varying pipe. The strength of thixotropy is described by advective and temporal Deborah numbers, which are the ratios of the structure response timescale to, respectively, the timescales of advection and the applied pressure gradient. In the regimes of 'weak thixotropy', in which the Deborah numbers are comparable to the small aspect ratio of the pipe, we follow the expansion method proposed by Pritchard et al. (2016) to obtain the effects of thixotropy and antithixotropy as perturbations to a generalised Newtonian flow. We present results for the Moore-Mewis-Wagner rheology. Pritchard et al. (2016) showed that in a widening channel (or a decelerating flow), thixotropy increases the fluid velocity near the centre of the pipe, while antithixotropy has the opposite effect. These results are generic for steady pipe flow. Unsteady pipe flow of an antithixotropic fluid is more complicated, and the shape of the velocity profile depends on some subtle dynamical balances. We show that for some rheological models the velocity perturbation for a strongly antithixotropic fluid mimics that for a thixotropic fluid. This casts doubt on whether generic statements can be made about antithixotropic lubrication flow. Numerical simulations agree with our solutions, and show that our lubrication approach is qualitatively accurate for flows in a range of aspect ratios.

Andrew I. Croudace, David Pritchard, Stephen Wilson
University of Strathclyde
andrew.croudace@strath.ac.uk,
david.pritchard@strath.ac.uk, s.k.wilson@strath.ac.uk

CP2
Complete Stabilization of Multi-Layer Radial Hele-Shaw Flows Using a Time-Dependent Injection Rate and the Associated Interface Motion

In this talk, we will discuss viscous fingering instabilities of multi-layer immiscible porous media flows within Hele-Shaw model in a radial flow geometry. We consider flows with both constant and variable viscosity fluids. It is a well-known result that a time-dependent injection rate can completely stabilize radial two-layer Hele-Shaw flows. We extend this result to three-layer flow by giving time-dependent upper bounds for the injection rate. We also present a numerical approach to simulating the interface motion within linear theory using the method of eigenfunction expansion. We compare these results with fully non-linear simulations. This work has been possible due to financial support from NPRP grant 08-777-1-141 through Qatar National Research Fund and the U.S. National Science Foundation grant DMS-1522782.

Craig Gin
Texas A&M University
cgin@math.tamu.edu

Prabir Daripa
Department of Mathematics
Texas A&M University
daripa@math.tamu.edu

CP2

The Stationary Navier-Stokes System with No-slip Boundary Condition on Polygons: Corner Singularity and Regularity

We study the stationary Navier-Stokes system with no-slip boundary condition on polygonal domains. Near each non-convex vertex the solution is shown to have a unique decomposition by singular and regular parts. The singular part is defined by a linear combination of the corner singularity functions of the Stokes type and the regular part is shown to have the $H^2 \times H^1$-regularity. The velocity vector is not Lipshitz continuous at nonconvex vertices and the pressure value is infinite there.

Jae Ryong Kweon
POSTECH(Pohang University of Science and Technology)
Korea
kweon@postech.ac.kr

CP2

The Influence of Tear Supply on Tear Film Formation During Upstroke

We simulate the tear film dynamics on a realistic blinking eye-shaped domain to examine the influence of the tear supply on the tear film formation during the upstroke. When the lids open, tear fluid from the upper meniscus and from under the upper lid is distributed onto the ocular surface to form a stable tear film. Because the current state-of-the-art instrumentation does not yet have the capability to image the tear film thickness over the entire front of the eye during the upstroke, especially near the upper lid, it is not fully understood how the tear supply impacts the tear film formation, and thus subsequent tear film thinning during the interblink. Using video of a blinking eye, we create a realistic moving eye-shaped domain by fitting the computational boundary curves to lid margins in the video. The evolution equation of the tear film thickness is derived using lubrication theory and includes the effects of viscosity and surface tension. By implementing a moving overset grid method, we examine how different models of tear supply, linked to lid motion and lid speed, affect the tear formulation and subsequent tear film breakup times. Our results are compared with prior modeling results and experimental observations.

Kara L. Maki
School of Mathematical Sciences
Rochester Institute of Technology
kmaki@rit.edu

William Henshaw
Rensselaer Polytechnic Institute
henshw@rpi.edu

Alex McManus
Rochester Institute of Technology
atm3702@rit.edu

Richard Braun
University of Delaware
rjbraun@udel.edu

Tobin Driscoll
University of Delaware
Mathematical Sciences
driscoll@udel.edu

CP2

Generalizing the Modified Buckley-Leverett Equation with Tcat Capillary Pressure

The Buckley-Leverett partial differential equation has long been used to model two phase flow in porous media. Applications include secondary oil recovery as well as contaminant flow in groundwater. In recent years, the PDE has been modified to include a rate-dependent capillary pressure constitutive equation. Known as dynamic capillary pressure, this constitutive equation describes the difference between pressures at the interface of the two fluid phases with an equilibrium pressure and a time-dependent term involving saturation of the water phase. More recently, thermodynamically constrained averaging theory (TCAT) has generalized the capillary pressure equation by including additional dependence on fluid properties. In this talk, we describe the changes in the Buckley-Leverett PDE that result from incorporating TCAT capillary pressure. Traveling wave analysis of the updated model uncovers both classical and nonclassical solution structures of the associated Riemann problem, when the initial condition of the PDE represents a jump discontinuity between the two fluids. Remarkably, and unlike the case of dynamic capillary pressure with quadratic relative permeability functions, nonclassical solutions involving an undercompressive shock now exist when the initial condition involves pure fluids.

Kimberly Spayd
Gettysburg College
kspayd@gettysburg.edu

CP2

Non-Classical Dispersive Shock Waves in Shallow Water: Theory and Experiments

In the 1950's and 1960's, experiments involving a thin film of water flowing at supercritical speed around an obstacle were conducted under the auspices of the "hydraulic analogy" to gas dynamics where two-dimensional, compressible shock waves described by the isentropic Euler equations were modeled as steady, shallow water flows. However, due to the dispersive nature of the flow, the wave patterns generated in water were, in fact, steady dispersive shock waves (DSWs), wholly different from their viscous shock wave counterparts in air. In this talk, the fifth order Korteweg-de Vries or Kawahara equation is derived as a model of the steady, supercritical, shallow water free surface when dispersion due to both capillary and gravity effects are in balance with nonlinear effects. Due to the presence of fifth order dispersive terms in the Kawahara equation, the dispersion relation can be non-convex, resulting non-classical dispersive shock structures, which are classified in detail. Experiments involving the aforementioned steady oblique DSWs are performed and are found to compare favorably with the model's predictions.

Patrick Sprenger
University of Colorado at Boulder
Patrick.Sprenger@Colorado.EDU

Mark A. Hoefer
Department of Applied Mathematics
University of Colorado at Boulder

hoefer@colorado.edu

CP3
Mathematical Modeling of Plants under Multiple Stressors

Plants, especially endangered species are usually a?ected by multiple stressors, including insects, and herbivores, environmental factors such as drought and heat, and other species. Here we present models based on systems of ordinary differential equations of two herbivores feeding (stressors) on the same plant species. The models incorporate several features: no competition between the herbivores, only intra-species competition, and intra as well as inter-species competition. In addition, the models integrate distinct types of multiple stressors: synergistic or antagonistic. We investigate conditions for coexistence of the tree. Our results suggest that to obtain stable coexistence solutions the model needs to incorporate significant herbivore species interaction: inter- or intra-species competition or both.

Maria Leite
University of South Florida at St Petersburg
Mathematics & Statistics
mcleite@mail.usf.edu

Benito Chen-Charpentier
Department of Mathematics
University of Texas at Arlington
bmchen@uta.edu

Orou Gaoue
University of Hawaii at Manoa
ogaoue@hawaii.edu

Folashade Agusto
Department of Ecology and Evolutionary Biology
University of Kansas
fbagusto@ku.edu

CP3
Analysis of a Mathematical Model of Pathogen Dynamics in Water Distribution Networks With Time Periodic and Aperiodic Flows

A water distribution network is system that aims to provide a safe water supply. Biological contamination of the system can occur by breach on pipes and several other factors, impacting the water quality. Frequently, microorganisms form biofilms on the interior surface of pipes, which are aggregates of microorganisms that adhere to solid surfaces through self secreted extra cellular polymeric substances. The presence of typically harmless drinking water biofilms can allow harmful bacteria to persist within the distribution network, possibly degrading water quality. In this talk, we analyze a mathematical model of the dynamics of non native bacteria with the native drinking water biofilm within a large network of pipes, for a time periodic and aperiodic flows. We analyze the dynamics of models using linear stability analysis with Floquet theory. For realistic water distribution systems, there exists a number of connections in the network making Floquet multipliers inefficient, to address this we develop an efficient algorithm for predicting the long-time behavior of the pathogen population within the network and prove mathematically these predictions are equivalent to results from Lyapunov and Floquet theory. The analytical results are validated using numerical simulations of the full non-linear system on a range of water distribution network sizes

Alvaro A. Ortiz Lugo
Phd Student
University of Cincinnati
ortizlaa@mail.uc.edu

CP3
Observation, Modeling and Computation of Algal Swimming and Photosynthesis

We model and analyze *Heterosigma akashiwo* as a model species for mixotrophic plankton. *H. akashiwo* is a swimming alga that can perform inefficient photosynthesis as well as graze on bacteria. It is also responsible for harmful algal blooms. Understanding their motion and behavior is crucial for anticipating the health of marine ecosystems. Observations of their behavior in a controlled setting reveals that *H. akashiwo* exhibit spatial patterns that evolve on a timescale of 10s of minutes. We present a mathematical model to explain the observed spatial patterns and cyclic behavior. The key mechanisms in the model are optical attenuation, phototaxis and photosystem excitation, degredation and repair. Photosystem degredation and repair are modeled as a relaxation oscillation. Taken together, they yield a dynamic swarming system with a spatially asymmetric interaction kernel.

Louis F. Rossi
University of Delaware
rossi@math.udel.edu

CP3
Mathematical Model of Pathogen Dynamics in a Water Distribution Network under Time-Constant Flow Conditions

In industrialized nations, the availability of potable water is provided through sophisticated water distribution systems that consists a network of pipes, pumping stations, reservoirs, and other components that deliver safe drinking water to consumers. Biological contamination of the water distribution system, due to factors such as a breach in a pipe or other causes, can have an adverse effect on water quality. In this talk, we discuss the development and analysis of mathematical model of the release of pathogenic bacterial species into the water distribution system. Bacteria within a water distribution system frequently form biofilms on the interior surfaces of pipes that pathogens can attach to and grow, possibly leading to the persistence of the pathogens within the network. This mathematical model is studied under time-constant using Lyapunov stability as well as numerical simulations. Frequently, water distribution networks have a significant number of connections, making direct calculations expensive so we developed and analyzed an efficient approach for predicting the long-time behavior of the pathogen population for large water-distribution networks. The analytical results are validated using numerical simulations of the full non-linear system on a range of water distribution network sizes.

Benjamin L. Vaughan, Sadiqah Al Marzooq, Alvaro Ortiz-Lugo
University of Cincinnati
vaughabn@ucmail.uc.edu,   almarzsa@mail.uc.edu,   orti-

zlaa@mail.uc.edu

CP3

Modeling Stripe Formation on the Body and Fins of Zebrafish

Zebrafish (Danio rerio) is a small fish with distinctive black and yellow stripes that form on its body and fins due to the interactions of different pigment cells. Working closely with the biological data, we present an agent-based model for these stripes that accounts for the migration, differentiation, an death of three types of pigment cells on the zebrafish body. We also explore stripe formation on the caudal fin, where bone rays and fin growth seem to help direct pigment cell placement. Both wild-type and mutated patterns will be discussed.

Alexandria Volkening, Bjorn Sandstede
Division of Applied Mathematics
Brown University
alexandria_volkening@brown.edu,
bjorn_sandstede@brown.edu

CP4

A Semi-Lagrangian Finite Difference Weno Scheme for Scalar Nonlinear Conservation Laws

For a nonlinear scalar conservation law in one-space dimension, we develop a locally conservative semi-Lagrangian finite difference scheme based on weighted essentially non-oscillatory reconstructions (SL-WENO). This scheme has the advantages of both WENO and semi-Lagrangian schemes. It is a locally mass conservative finite difference scheme, it is formally high-order accurate in space, it has small time truncation error, and it is essentially non-oscillatory. The scheme is nearly free of a CFL time step stability restriction for linear problems, and it has a relaxed CFL condition for nonlinear problems. The scheme can be considered as an extension of the SL-WENO scheme of Qiu and Shu [J. Comput. Phys., 2011] developed for linear problems. The new scheme is based on a standard sliding average formulation with the flux function defined using WENO reconstructions of (semi-Lagrangian) characteristic tracings of grid points. To handle nonlinear problems, we use an approximate, locally frozen trace velocity and a flux correction step. A special two-stage WENO reconstruction procedure is developed that is biased to the upstream direction. A Strang splitting algorithm is used for higher-dimensional problems. Numerical results are provided to illustrate the performance of the scheme and verify its formal accuracy. Included are applications to the Vlasov-Poisson and guiding-center models of plasma flow.

Todd Arbogast
University of Texas at Austin
arbogast@ices.utexas.edu

Chieh-Sen Huang
National Sun Yat-sen University
Kaohsiung, Taiwan
huangcs@math.nsysu.edu.tw

Chen-Hui Hung
Air Force Academy
Kaohsiung, Taiwan

hungch@math.nsysu.edu.tw

CP4

The Semi-Lagrangian Discontinuous Galerkin Method on Modern Computer Architectures

To numerically solve the Vlasov equation is a challenging task due to the high dimensional phase space and the desire to conserve physically relevant invariants. Time splitting schemes combined with a cubic spline based semi-Lagrangian approach have been extensively used in the literature. However, spline interpolation is a global algorithm and is thus not well suited for modern computer architectures. More recently, the semi-Lagrangian discontinuous Galerkin scheme has been introduced (see [N. Crouseilles et al., Proc. of ESAIM, 2011], [J. Rossmanith, D. Seal, J. Comput. Phys., 230, 2011], [J. Qiu, C. Shu, J. Comput. Phys., 230(23), 2011]). Its mathematical convergence [L.E., A. Ostermann, SIAM J. Numer. Anal., 52(2), 2014] and its favorable conservative properties [L.E., arXiv:1601.02280] have been studied. In the present talk we report on recent results that show that our template based dimension independent semi-Lagrangian discontinuous Galerkin implementation can scale to tens of thousands of cores [L.E., Comput. Phys. Commun., 202, 2016]. Furthermore, we introduce a mixed precision implementation that exploits the particular structure of this numerical method and is so able to decrease memory consumption and increase performance without sacrificing, e.g., conservation of mass up to double precision accuracy [L.E., Proc. of HPCS, 2016]. In this context results on GPUs and on the Intel Xeon Phi are presented that demonstrate performance close to the hardware limit.

Lukas Einkemmer
University of Innsbruck
lukas.einkemmer@uibk.ac.at

CP4

An Approximate Inverse Preconditioner for Spatial Fractional Diffusion Equations with Piecewise Continuous Coefficients

In this paper, we study the discretized linear systems arising from the space-fractional diffusion equations with piecewise continuous coefficients. Using the implicit finite difference scheme with the shifted Grünwald discretization, the resulting linear systems are Toeplitz-like which can be written as the sum of a scaled identity matrix and two diagonal-times-Toeplitz matrices. Standard circulant preconditioners or the existing approximate circulant-inverse preconditioner do not work for such Toeplitz-like linear systems since the discontinuous diffusion coefficients cannot be well approximated by interpolation polynomials. The main aim of this paper is to propose a new approximate circulant-inverse preconditioner to handle the fractional diffusion equations with discontinuous coefficients. Our idea is to approximate the eigenvalues of circulant matrices by the interpolation formula instead of approximating the diffusion coefficients as the existing algorithms do. Therefore, the discontinuity of the diffusion coefficients does not influence the efficiency of the preconditioner. Theoretically, the spectra of the resulting preconditioned matrices are shown to be clustered around one, which can guarantee the fast convergence rate of the proposed preconditioner. Numerical examples are provided to demonstrate the effectiveness of our method.

Zhi-Wei Fang

Department of Mathematic
University of Macau
fzw913@yeah.net

Hai-Wei Sun, Hui-Qin Wei
Department of Mathematics
University of Macau
hsun@umac.mo, mb55477@umac.mo

CP4

A Numerical Study on the Time Parallel Approach for the Semi-Linear Wave and Dirac Equations

Highly time-dependent problems in physics have been addressed to answer important phenomena such as formation of singularity in spacetime and structure of quantum system. Because of complexity of this problem, successful numerical simulations are required to interpret these systems. In this talk, we will present a time parallel approach for linear, semi-linear wave, and Dirac equations. The time parallel method is a fully implicit approach based on time additive Schwarz preconditioner for a Krylov subspace method and space time finite element methods. The results show that the proposed numerical procedures can be extended to higher dimension and resolution simulations for physically interesting problems. The time parallel algorithm is implemented through PETSc (Portable, Extensible, Toolkit for Scientific Computation) developed by Argonne National Laboratory and the standard MPI infrastructure. The performance test results against number of processors and different dimensions will be discussed.

Jung-Han Kimn
Mathematics & Statistics
South Dakota State University
jung-han.kimn@sdstate.edu

Hyun Lim
Department of Physics and Astronomy
Brigham Young University
hyun.lim@byu.net

Nicholas W. Stegmeier
South Dakota State University
nicholas.stegmeier@jacks.sdstate.edu

CP4

High Order Monotone LPS Scheme Based on Bernstein-Bezier Finite Elements for Nonlinear Hyperbolic Systems

An arbitrarily high order monotone local projection stabilization (LPS) scheme is proposed for nonlinear hyperbolic systems and highly coupled problems. We make use of the Bernstein-Bezier finite element space. The positivity and partition of unity properties of the Bernstein basis makes them appealing for problems that require positivity preservation. We consider a stabilization approach in which low order minimal dissipation is added to the semi-discrete for of the problem. The result is a semi-discrete form which satisfies the system LED condition. Then element based LPS limiters are introduced to make the scheme high resolution. To deal with phase errors, we add background high order dissipation such as SUPG. The stabilized semi-discrete scheme can then be discretized in time using various time integrators. Numerical studies are done to illustrate the performance of the scheme with various scalar

problems and with shock hydrodynamics problems.

Sibusiso Mabuza, John N. Shadid
Sandia National Laboratories
smabuza@sandia.gov, jnshadi@sandia.gov

Dmitri Kuzmin, Christoph Lohmann
Dortmund University of Technology
kuzmin@math.uni-dortmund.de,
christoph.lohmann@mathematik.tu-dortmund.de

CP4

Direct Fem Simulation of Multi-Phase Turbulent Flow

In this seminar we will present an overview of the Direct FEM methodology for turbulent flow and recent new developments toward multi-phase flow with applications in marine energy, and parallel-in-time simulation. Our methodology is based on a piecewise linear approximation in space and time and with a numerical stabilization in the form of a weighted least squares method based on the residual. The methodology has several unique aspects which we hope can advance the field in new directions: 1. The incompressible Navier-Stokes Equations (NSE) are discretized directly, without applying any filter. Thus, the method does not approximate any Large Eddy Simulation (LES) filtered solution, but is instead an approximation of a weak solution, satisfying the weak form of the NSE. 2. For this method, we have a posteriori error estimates of quantities of interest with respect to a weak solution, which form the basis for our adaptive mesh refinement algorithm. The a posteriori error estimates are based on the solution of an associated adjoint problem with a goal quantity (such as a drag coefficient) as data. 3. We model turbulent boundary layers by a slip boundary condition which is a good approximation for small skin friction stress, which gives enormous savings in computational cost by not having to resolve a very thin boundary layer.

Margarida Moragues Ginard
Basque Center for Applied Mathematics
mmoragues@bcamath.org

Tania Bakhos
Basque Center for Applied Mathematics
tbakhos@bcamath.org
tbakhos@bcamath.org

Daniel Castañón
Basque Center for Applied Mathematics
dcastanon@bcamath.org
dcastanon@bcamath.org

Johan Hoffman
Royal Institute of Technology KTH
jhoffman@kth.se

Johan Jansson
School of Computer Science and Communication
KTH Royal Institute of Technology
jjan@kth.se

Ezhilmathi Krishnasamy
Basque Center for Applied Mathematics
ekrishnasamy@bcamath.org

Massimiliano Leoni
Basque Center for Applied Mathematics

KTH Royal Institute of Technology
mleoni@bcamath.org

Laura Saavedra
Polytechnic University of Madrid
laura.saavedra@upm.es

CP5
Discrete Homogenization Theory for Random Walks on Graphs Embedded in the Euclidean Space

We study the homogenization limit of a biased random walk on a periodic graph embedded in the multidimensional Euclidean space. Our model is inspired by the problem of solute diffusion in an aqueous polymer environment. Prediction of effective solute diffusivity in aqueous polymer environments enables the design of polymer-based drug and protein delivery devices as well as cell scaffolds for tissue engineering, among other applications. Our rationale for considering a random walk on a graph is to account for the fact that the mean path length of a diffusing solute may not be much smaller than the finescale length of the structures of interest. When the finescale length of interest is only a few nanometers, as in the case of polymer gel networks, the case for our starting point is quite strong. First, the effective diffusivity is formally derived via an intuitive approach that assumes the probability mass function of the random walk admits an asymptotic expansion. This expansion yields a set unit-cell problems that must be solved in order to compute the effective diffusivity. Next, the effective diffusivity is rigorously derived by leveraging the martingale functional central limit theorem. The main results are 1) agreement between the formal and rigorous derivations and 2) a mathematical formula for the effective diffusivity in terms of the embedded graph and the solutions to the unit-cell problems.

Preston Donovan, Muruhan Rathinam
University of Maryland, Baltimore County
pdonovan@umbc.edu, muruhan@umbc.edu

CP5
Minor Set Covers of Biclique Graphs

The emergence of non-von Neumann computing architectures has expanded the way we think about the task of computer programming. For adiabatic quantum optimization, programming a quantum annealer relies on mapping a target graph $(\mathcal{G})$ to a minor of a fixed hardware graph $(\mathcal{U})$. The hardware graph has an associated set of minors which is large and searching over the entire set is resource and time intensive. To expedite this search, we propose using a lookup table of stored embeddings, and recently introduced the concept of a *minor set cover* [1] to provide the table keys. There exist graphs where a finite subset of minors will effectively cover the entire set of the graph's minors: any minor of the graph is contained as a set member or contained within a set member as a subgraph. Using a minor set cover, the task of minor embedding can be executed over a reduced search space, only a subset of minors need to be generated for a given graph, and the embeddings can be stored for later use. We present results for biclique graphs $K_{N,N}$. These graphs have minor set covers with qualities which aid in efficient searching of the set, such as: clique number, degree distribution, graph size and graph order.
[1] Hamilton, Kathleen E., and Travis S. Humble. "Identifying the minor set cover of dense connected bipartite

graphs via random matching edge sets.' arXiv preprint arXiv:1612.07366 (2016).

Kathleen Hamilton
Oak Ridge National Laboratory
Complex Systems Division
k8hamilton@gmail.com

Travis Humble
Oak Ridge National Laboratory
humblets@ornl.gov

CP5
Spectral Clustering of Signed Graphs Revisited

Classical spectral clustering is based on a spectral decomposition of a graph Laplacian, obtained from a graph adjacency matrix representing positive graph edge weights describing similarities of graph vertices. In signed graphs, the graph edge weights can be negative to describe disparities of graph vertices, for example, negative correlations in the data. Negative weights lead to possible negative spectrum of the standard graph Laplacian, which is cured by defining a signed Laplacian. We follow [A. Knyazev, Signed Laplacian for Spectral Clustering Revisited, https://arxiv.org/abs/1701.01394, 5 Jan 2017] to compare the standard and signed Laplacians and numerically evaluate LOBPCG [A. Knyazev, Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method. SIAM Journal on Scientific Computing. 23 (2): 517, 2001], for spectral clustering of signed graphs.

Andrew Knyazev
Mitsubishi Electric Research Laboratories (MERL)
knyazev@merl.com

CP5
Topological Methods and Classification of Complex Patterns

Complex spatial-temporal patterns can be difficult to characterize quantitatively, but examples of such patterns are ubiquitous. For example, the anisotropic Kuromoto-Sivashinky equation which has been derived to model pattern-forming systems driven far from equilibrium in a wide array of applications. In seeking to understand the mechanisms of pattern formation, studying the effect of parameters on the formation and evolution of complex spatio-temporal patterns offers valuable insight into underlying mechanisms driving the system. However, determining these parameters can be difficult and computationally expensive. We believe that the parameters influence the dynamic data in a way that is detectable by persistent homology. Using a finite-dimensional vector representation of persistence diagrams called persistence images, we are able to leverage machine learning techniques to classify data by parameters and to consider the temporal evolution of the pattern. The reduction of the dynamic data using persistent homology still retains a remarkable amount of information that is useful for parameter classification and for temporal and we are able to achieve good classification results for simulated data.

Rachel Neville
Colorado State University
neville@math.colostate.edu

Patrick Shipman

Department of Mathematics
Colorado State University
shipman@math.colostate.edu

CP5
An Algorithm for Creating Synthetic, Differentially Private Database Tables from Large Database Tables

We have developed an algorithm for the development of synthetic, differentially private tables from database tables requiring anonymization using a differentially private, Bayesian classification algorithm. We characterize the privacy characteristics and performance of the algorithm.

Jeffrey S. Saltzman
Cottonwood Analytics
jeffsaltzman@cottonwoodam.solutions.com

CP5
Graph Representations of Fracture Networks for Predicting Flow and Propagation

The behavior of fractured systems is governed by the properties and interactions at the micro-scale. Retaining information about the micro-structure such as fracture length, orientation, aperture and connectivity in mesh-based computational models results in solving for millions to billions of degrees of freedom and quickly renders the problem computationally intractable. Our approach depicts fracture networks graphically, by mapping fractures to nodes and intersections to edges, thereby greatly reducing computational burden. This talk focuses on two specific applications involving flow through static fractures and propagation of fractures. We apply principles of network transport and dynamic graph theory to advance predictive capabilities for these two applications using the corresponding reduced graph-based models.

Gowri Srinivasan
T-5, Theoretical Division, Los Alamos National
Laboratory
gowri@lanl.gov

Hari Viswanathan
Los Alamos National Laboratory
Earth and Environmental Sciences Division
viswana@lanl.gov

Aric Hagberg
Los Alamos National Laboratory
hagberg@lanl.gov

Jeffrey Hyman
Los Alamos National Laboratory
Earth and Environmental Sciences Division
jhyman@lanl.gov

Daniel O'Malley
Los Alamos National Laboratory
omalled@lanl.gov

Satish Karra
Los Alamos National Laboratory
Earth and Environmental Sciences Division
satkarra@lanl.gov

Esteban Rougier, Bryan Moore, Maruti Mudunuru
Los Alamos National Laboratory
erougier@lanl.gov, bryanmoo@lanl.gov, maruti@lanl.gov

CP6
How Boundaries Shape Chemical Delivery in Microfluidics

We present the results of a combined theoretical, computational and experimental study of the dispersion of a passive scalar in laminar shear flow through rectangular and elliptical channels. We show through Monte Carlo simulation, asymptotic analysis and experiments that the cross-sectional aspect ratio sets the sign of the average skewness at long times (relative to the Taylor diffusion timescale) which describes the longitudinal asymmetry of the tracer distribution. Universally, thin channels (aspect ratio $\ll 1$) result in negative average skewness, whereas thick channels (aspect ratio ~ 1) result in positive average skewness. Our analysis also allows us to define a "golden aspect ratio which separates thin from thick channels, the value of which is remarkably similar for both the rectangle and the ellipse. Further, by examining the median of the cross-sectionally averaged distribution, we establish that negative skewness correlates with solutes arriving with sharp fronts followed by a tapering tail. Future directions and possible microfluidics applications will be discussed.

Francesca Bernardi, Manuchehr Aminian
UNC
bernardi@live.unc.edu, aminian@live.unc.edu

Roberto Camassa
University of North Carolina
camassa@amath.unc.edu

Daniel Harris, Richard McLaughlin
University of North Carolina at Chapel Hill
dmh@email.unc.edu, rmm@email.unc.edu

CP6
On the Modeling of Displacement of Non-Newtonian Fluids in Porous Media Flows

Current work on the development, analysis and implementation of non-Newtonian models for porous media flow will be discussed. In this connection, we will also consider prototype models within Hele-Shaw approximation and present some preliminary results. This work has relevance for modeling chemical enhanced oil recovery processes. This work has been possible due to financial support from the U.S. National Science Foundation grant DMS-1522782.

Prabir Daripa
Texas A&M University
Department of Mathematics
prabir.daripa@math.tamu.edu

CP6
Numerical Investigation on the MVG Controlled Shock Wave Vortex Rings Interaction

A wedge-shaped micro vortex generator is placed on a flat plate over which a turbulent boundary layer at Mach number 2.5 is developed. The interaction between an oblique shock wave and high-speed vortex rings in the MVG controlled ramp flow is investigated by using a high order implicit large eddy simulation with the fifth order bandwidth

optimized WENO scheme. The vortical structures are visualized using the Omega identification method proposed by the UTA researchers. The vortex rings propagate downstream and interact with the separation shock, eventually distorting the structure of the shock. By tracking several typical vortex rings before, when and after they pass through the shock front, the quantitative changes of flow properties are studied in detail. During this process, the vortex rings maintain the topology well after penetrating the shock but rotate not as fast as before, the shock gets distorted when hit by rings and moves back and forth, and a number of weak shocks exist around ring heads in the downstream. The shock ring interaction provides an insight in understanding the presence of the low-frequency unsteadiness in separation shock motions. The pulsation of the separation bubble is found to be related to the vortex ring propagation.

Yinlin Dong, Chaoqun Liu
University of Texas at Arlington
yinlin@uta.edu, cliu@uta.edu

CP6
A Stable Semi-Implicit Finite Element Method for a Dynamic Interface Problem on An Unfitted Mesh

Solving a time-dependent PDE with a dynamic interface is very computationally expensive, particularly on a complicated domain. The problem becomes even more time-consuming when one must fit a new mesh to the domain each time the interface moves. When using finite element methods (FEM) to solve the problem, this can be avoided by using CutFEM to separate the mesh structure from the domain. Using a time-dependent CutFEM method we solve the immersed boundary method on a structured mesh with optimal convergence. We introduce a semi-implicit method to solve this problem, prove it's stability, and apply the resulting algorithm to an elementary cell motility model.

Kyle G. Dunn
Worcester Polytechnic Institute
36kdunn@gmail.com

Marcus Sarkis
Worcester Polytechnic Institute
Instituto de Matematica Pura e Aplicada (Brazil)
msarkis@wpi.edu

Roger Lui
Worcester Polytechnic Institute
rlui@wpi.edu

CP6
Recent Studies on Vortex Dynamics and Its Applications to Biological Problems

I want to take the chance in this talk to present my recent studies on vortex dynamics and its applications to biological problems. The first project is about viscous flow past a plate/wedge, and the goal is to study on the starting vortex evolutions near a sharp edge at an early and medium time. In this work, various scaling laws regarding the shed circulation, vortex core trajectory are revealed. The second project is about simulating fish schools, and the goal is to investigate the effects of the hydrodynamic interactions among groups of swimmers. We have found that there is inter-spacing selection in forward swimming speed. The first two projects use finite-difference schemes and I will

also report on work that aims to develop an improved vortex method to make it more efficient in resolving delicate vortex structures.

Ling Xu
University of Michigan, Ann Arbor
lingxu@umich.edu

CP7
Modelling and Design of Nano-Structures: Multi-layer Nanoplasmonics Configurations:

Nanoplasmonics forms a major part of the field of nanophotonics, which explores how electromagnetic fields can be confined over dimensions on the order of or smaller than the wavelength. Initiated in 1902 by R.W. Wood with the discovery of grating anomalies, this phenomenon has attracted significant attention over the last hundred years. We believe that state-of-the-art computational thinking can be used to dramatically improve the design process for multi-layered nanostructured optical materials. The configuration will composed of a thin layer of noble metal with depth larger than skin depth of the material, buried into different epoxies on top (glass/polymer substrate) and the bottom (liquid/water/blood). The use of such can only proceed at this time, when fabrication processes have advanced to the level of allowing for very fine control of metallic patterns (on the order of 1 to 2 nm). This, in turn, justifies the use of accurate schemes that will replace current practices which still rely largely on old-fashioned and inaccurate techniques (such as the FDTD, finite element and integral equation methods) each one of these is limited in accuracy and/or efficiency, rendering them of limited use in virtual design. On the other hand, the schemes we describe are based on high-order (spectral) treatment of the (integral-equation formulation of the) mathematical models and they can thus deliver highly accurate solutions in fast computational times.

Harun Kurkcu
Gulf University for Science and Technology
kurkcu.h@gust.edu.kw

CP7
Dynamic Optimization of Polymer Grade Transitions with Molecular Weight Distribution Models

Molecular weight distribution (MWD) is a crucial quality index that directly determines end-use polymer properties. The needs for fast and economical dynamic grade transition policies motivate dynamic optimization with detailed population balance polymer reaction models. Conventionally, a Flory-Schulz distribution with a small-scale moment model has been used to calculate MWD, but it is valid only under steady state or pseudo steady state assumptions. This talk develops a full population balance model formulated using orthogonal collocation on finite elements (OCFE) for both the MWD and time, without any limiting assumptions. In the OCFE formulation, the population balance equations of polymer chains are satisfied exactly at the collocation points on the chain length domain, the solutions of which are used to reconstruct MWD directly. This approach is demonstrated on an industrial high-density polyethylene (HDPE) slurry process with a continuous stirred-tank reactor and several auxiliary units. A detailed mathematical model is developed to track the behavior of the entire plant with liquid and vapor recycles. First, we consider a steady-state optimization problem with specified MWDs. Here, a comparison

with a Monte Carlo method demonstrates the accuracy of OCFE. Next, a dynamic grade transition problem will be presented, where a direct transcription optimization approach is applied to solve this problem after fully discretizing state and control variables.

Yannan Ma
Carnegie Mellon University
nightingale_zju@126.com

Xi Chen
Zhejiang University
xi_chen@zju.edu.cn

Lorenz Biegler
Carnegie Mellon University
Department of Chemical Engineering
lb01@andrew.cmu.edu

CP7
Mathematical Modeling of Nanofluid Based Solar Collectors

The solar energy industry has experienced phenomenal growth in recent years due to both technological improvements resulting in cost reductions and government policies supportive of clean technology and renewable energy development. In this contributed talk we propose an approximate analytic solution to a three-dimensional model for the efficiency of a nanofluid based concentrating parabolic trough solar collector. Our model consists of a system of partial differential equations describing the conservation of mass, momentum and energy. A heat source term is obtained via the radial flux integral, which is highly non-linear with respect to wavelength due to the spectral-dependent fluid and nanoparticle indices of refraction and absorption. To make analytic progress we introduce an approximate power-law function for the radial flux. The resulting solution is used to investigate the efficiency of the collector subject to variation in model parameters. Our solution permits optimization of design parameters such as particle loading and particle type, solar absorption characteristics of the fluid, channel dimensions, the inlet temperature, and fluid flow conditions.

Gary J. O'Keeffe, Sarah Mitchell
University of Limerick
Ireland
gary.okeeffe@ul.ie, sarah.mitchell@ul.ie

Tim G. Myers
KAIST
South Korea
tmyers@crm.cat

Vincent Cregan
Centre de Recerca Matemàtica
Spain
vcregan@crm.cat

CP7
Optical Beams Interaction at the Interface of Two Nonlinear Optical Media

We studied a computationally intensive problem of light beams interaction at the interface and waveguide of nonlinear optical media. The beam dynamics is simulated by the beam propagation method and the particle theory is applied to understand the problem analytically. The numerical simulations agree with the results of analytical model. The trapped beam at the interface acts as a power controllable switch to reflect or transmit the incident beam at the interface. This results can be used to develop a device in signal switching.

Rajah P. Varatharajah
North Carolina A&T State University
rajah@ncat.edu

CP7
Instability and Patterns of Active Suspensions of Liquid Crystals

We first present a continuum model for active, anisotropic fluids arising from biological and materials science applications, which is derived from the kinetic model using closure rules. The equations include transport equations for the polarity vector and the local concentration, as well as the Navier-Stokes equations. Then we examine the linear stability of the isotropic state and the constant polarity equilibrium of active suspensions of liquid crystals. Numerical simulations based on this model reveal several excitable patterns, and a complete phase diagram of stable attractors is produced in the active and polarity-strength parameter space.

Robert A. Williams
Old Dominion University
ra1willi@odu.edu

Ruhai Zhou
Department of Mathematics and Statistics
Old Dominion University
rzhou@odu.edu

CP8
Permutation Complexity Measures for Time-Series Data

Combinatorial methods, such as permutation entropy, have become important tools for robustly measuring the complexity of dynamical systems. The temporal aspect of time series data allows us to analyze the distribution of permutations of length n that appear as the relative orderings of each set of n consecutive points. In this presentation, we consider time series t_i, generated as the sum of i.i.d. random variables X_i. In 2015, Martinez showed that certain combinatorial relations between the permutations determine equivalence classes that must appear with equal proportions in the t_i for any choice of X. This complements earlier work of Bandt, Keller, and Pompe on forbidden patterns in iterated functions and of Amigo and Elizalde on shift systems. Motivated by these results, we define two new complexity measures for real-valued, time series data. The first measure uses the results of Martinez directly to compare the deviance of empirical permutation distributions from the theoretical expectation. The second measure compares the transition probabilities between sequential permutations in the time series. This is equivalent to representing time series by an associated random walk on S_n, allowing for the application of additional combinatorial techniques. As a model for financial time series, we provide analytical results for uniform random walks with drift, expressing their distribution of permutations in terms of hyperplane arrangements.

Daryl R. Deford, Katherine Moore

Dartmouth College
Department of Mathematics
daryl.r.deford.gr@dartmouth.edu, katherine.e.moore.gr@dartmouth.edu

CP8

A Global Nonlinear Dimensionality Reduction Framework Using Smooth Geodesics

Existing dimensionality reduction methods adept at revealing hidden underlying manifold of high-dimensional data and producing a low-dimensional representation. However, the smoothness of this manifold that relies on the method is not promising. In fact, the embedding performed using such non-smooth manifold might loose the topology of the manifold and thereby produces an unfaithful embedding. Here, we propose a framework for nonlinear dimensionality reduction that replicates the manifold in terms of smoothing geodesics. We create a network structure for a given high-dimensional data using a neighbor search and then produce geodesics between points followed by fitting a smoothing spline over points on each geodesic. The robustness of this approach for noisy and sparse data sets is justified by examples.

Kelum D. Gajamannage, Randy Paffenroth
Worcester Polytechnic Institute
dineshhk@clarkson.edu, rcpaffenroth@wpi.edu

Erik Bollt
Clarkson University
bolltem@clarkson.edu

CP8

Price of Non-Iidness and Minimax Coincidence

In most real world learning applications it is not known how well the data or nontrivial transformations thereof conform to the assumptions made in theory. "Independent and identically distributed' for example is a standard assumption that is often violated in practice. Moreover, when past data may be misleading or otherwise unrepresentative of the future, it is impossible to learn if the data is close to being independent and identically distributed. "Adversarial' in contrast imposes no probabilistic constraints; instead an adversarial process can deterministically attempt to mislead or otherwise confuse the statistician. Of course adversarialism has its own limitation: that of being pessimistic. Despite the disparity between non-IIDness and adversarialism, for a given application it may not be known which better approximates the data. Fortunately, in many settings learning under adversarialism is not much harder than learning under stationary, that is the minimax values only differ by a constant factor (**minimax coincidence**). In particular, I derive a lower bound of $\frac{\min\left(\sqrt{T}, \sqrt{\ln(N)}\right)}{32} \sqrt{T}$ and non-asymptotic minimax coincidence in the experts setting with absolute loss and similar settings with L^1-norm loss.

Michael Spece
Carnegie Mellon University
spece@cmu.edu

CP8

Estimation of Henze-Penrose Divergence Measures

The information divergence is a measure of the difference between two probability distributions. Information divergence is relevant to many applications ranging from machine learning, statistics and information theory. For instance, f-divergence measures like Chernoff, Batacharria and Mahalanobis divergence can be used to provide bounds on the minimum binary classification probability of error for classification problems. Recently tighter bounds on the Bayes error rate in terms of Henze-Penrose divergence have been derived. This motivates the problem we consider in this paper: empirical estimation of Henze-Penrose divergence when the distributions are unknown but random samples from these distributions are available. An estimation method proposed by Friedman and Rafsky derives from the Euclidean minimal spanning tree (MST) that spans the merged random samples. In this paper we give rates of convergence for their estimator. Let the two samples consist of m and n points, respectively, drawn from multivariate smooth densities f_0 and f_1 and assume that these densities have common compact support and are smooth with Hölder smoothness parameter η. Then the almost sure convergence rate is $O(l^d(m+n)^{-\eta/d} + O(l^d(m+n)^{-1/2}) + O(l^{-d\eta})$ for $d \geq 4$. By studying the bias and variance rate, we provide a minimax optimal choice of tuning parameters for optimizing mean square error (MSE). These results are validated experimentally.

Salimeh Yasaei Sekeh, Morteza Noshad
EECS Department, University of Michigan, Ann Arbor
salimehy@umich.edu, noshad@umich.edu

Kevin Moon
Genetics and Applied Math Departments,Yale University
kevin.moon@yale.edu

Alfred Hero
University of Michigan
hero@umich.edu

CP9

Inferring Clogging Mechanisms from the Spreading of a Particle-Laden Fluid on a Porous Membrane

We consider the spreading of a gravity current carrying identical, neutrally buoyant particles on a thin membrane with uniform pores. Due to the drainage of the fluid through the membrane, the particles will clog the membrane and reduce its permeability. Depending on the size of the particles and the geometry of the pores of the membrane, different clogging mechanisms are observed: particles with diameters greater than that of the pores are retained at the surface, while smaller particles may accumulate within the membrane. These different clogging mechanisms lead to different rates for reducing the permeability of the membrane. In this talk, we show how we can infer the clogging mechanisms based on measuring the spreading speed of the front of the gravity current even if the concentration of the particles in the fluid is unknown. Modelling the spreading of the liquid using the porous medium equation with imbibition, we show that the influx needed to maintain a constant speed of the front depends uniquely on the blocking mechanism. Using asymptotic analysis, we show that this in turn can be exploited with a bisection method to then infer the blocking mechanism.

Armin U. Krupp
Mathematical Institute
University of Oxford
Armin.Krupp@maths.ox.ac.uk

Ian Griffiths, Colin Please
University of Oxford
ian.griffiths@maths.ox.ac.uk, colin.please@maths.ox.ac.uk

CP9
Stability of Oscillatory Rotating Boundary Layers

Some of the most popular applications of fluid mechanics come in aerodynamics, and methods of laminar flow control on swept wings have become increasingly important over the past few decades; especially with the global emphasis on emissions reduction. Another reason for the recent development of this field is the availability of high-performance computers, meaning calculations that would have been impossible only a decade ago can now be performed quickly on a workstation. With instability mechanisms in common with a swept wing, the rotating disk has long been considered as a valid approximation to this flow and is also far more amenable to experiments. The experimental setup for a rotating disk study requires a much smaller space and much less expensive equipment than the wind tunnel required for a swept wing experiment. For this reason, there are a wealth of experimental and theoretical studies of the rotating disk boundary layer and this talk will extend these established results. A recent study by Thomas et. al. [Proc. R. Soc. A (2011) 467, 2643-2662] discusses adding an oscillatory Stokes layer to a channel flow and shows some stabilising results. We present a similar modification to the rotating disk configuration by way of periodic modulation and provide results from both direct numerical simulations and local eigenvalue analyses showing a stabilising effect.

Scott N. Morgan
Cardiff University
MorganSN@cardiff.ac.uk

CP9
Coupling Effects Between An Applied Electric Field and Thermal Fluctuations in Dilute Electrolyte Solutions

We use fluctuating hydrodynamics to study the macroscopic consequences of applying an electric field to a dilute electrolyte solution, in the presence of fluid thermal fluctuations. By deriving the theoretical expressions of the structure factors of the velocities and local charge densities, we show in particular that the coupling between the local charge fluctuations and the applied field leads to a convective form of charge transport. This occurs in addition to electrodiffusion. We quantitatively evaluate the additional charge fluxes and show that, in very dilute solutions, this electroconvective charge transport is not negligible and results in a form of enhanced electric conductivity. Furthermore, electrostatic Lorentz force due to concentration fluctuations appears as a non-isotropic noise term in the momentum equation, which results in increased velocity fluctuations. Finally, we validate our theoretical findings using computational results obtained with finite volume simulations of the fluctuating equations [Peraud et al., Low Mach number fluctuating hydrodynamics for electrolytes, Physical Review Fluids, 1, 074103 (2016)], and we discuss the case of the electroneutral limit. Our results provide an additional example showing that thermal fluctuations are not only important for modeling small scale problems, but also have important macroscale implications that deterministic approaches cannot address.

Jean-Philippe M. Peraud

CCSE
Lawrence Berkeley National Laboratory
jperaud@lbl.gov

Andy Nonaka
Lawrence Berkeley National Laboratory
ajnonaka@lbl.gov

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

Alejandro Garcia
San Jose State University
algarcia@algarcia.org

CP9
Fouling of a Filter Membrane with Complex Microstructure: A Simplified Mathematical Model

Membrane filters are in widespread industrial use, and mathematical models to predict their efficacy are potentially very useful, as such models can suggest design modifications to improve filter performance and lifetime. Many models have been proposed to describe particle capture by membrane filters and the associated fluid dynamics, but most such models are based on a very simple structure in which the pores of the membrane are assumed to be simple circularly-cylindrical tubes spanning the depth of the membrane. Real membranes used in applications usually have much more complex geometry, with interconnected pores which may branch and bifurcate. Pores are also typically larger on the upstream side of the membrane than on the downstream side. We present an idealized mathematical model, in which a membrane consists of a series of bifurcating pores, which decrease in size as the membrane is traversed. Feed solution is forced through the membrane by applied pressure, and particles are removed from the feed either by sieving, or by particle adsorption within pores (which shrinks them). Thus the membrane's permeability decreases as the filtration progresses, ultimately falling to zero. We discuss how filtration efficiency depends on the characteristics of the branching structure.

Pejman Sanaei, Linda Cummings
New Jersey Institute of Technology
ps468@njit.edu, linda.cummings@njit.edu

CP9
Traffic Flow with Lane Changing

Traffic flow may be described by microscopic particle-like models or macroscopic fluid-like models. The latter models begin by stating car mass conservation, and naturally result in a hyperbolic conservation law for the car density. Velocity-density closure is required and traffic conditions considerations may lead to different closure laws, also referred to as fundamental diagram in traffic flow community (see for example Lighthill-Whitham 1955, Richards 1956). More recently, 2x2 systems have been proposed, where the additional equation governs car velocity and models car acceleration (for example Aw-Rascle 2000, Zhang 2002). This

talk will begin by discussing aspects of single lane traffic flow including velocity-density closures and various acceleration models in 2x2 systems. The models will then be generalized to describe multilane traffic with lane changes, describing mass exchanges between lanes, velocity acceleration/deceleration effects and response time. Lane changing is of particular interest in congested flows, and may give insight into flow phenomena such as the formation of bottlenecks.

Jiah Song
University of Michigan
jiahsong@umich.edu

Smadar Karni
University of Michigan
Department of Mathematics
karni@umich.edu

CP9

Corner Wetting and Drop Geometry During the Vapor-Liquid-Solid Growth of Facetted Nanowires

We consider the corner wetting of faceted nanowires in the context of vapor-liquid-solid growth of nanowires. In particular, we numerically determine the equilibrium shape of a liquid drop on top of wires of hexagonal cross section. In general, for a fixed contact angle the drop contact line approaches the corner as a function of increasing drop volume. The behavior of the liquid surface near the corners of the wire is nearly singular, and we determine the scaling behavior for the drop shape in the vicinity of the corner. A key result for nanowire growth is that for a range of contact angles there is no equilibrium drop shape that completely wets the corner because large drops violate the edge spillover condition before the corners are wetted. Finally, we show that even though the drop has near-singular behavior near the corners, the macroscopic drop shape can be determined from geometric considerations.

Brian J. Spencer
State University of New York at Buffalo
Department of Mathematics
spencerb@buffalo.edu

CP10

Membrane Thinning during Deformation

The cell membrane is a complex and interesting structure consisting of two monolayers of lipid molecules. Membranes are continuously subjected to deformations, which has led to them becoming a subject of intense study from a theoretical viewpoint. A good example of this is the mechanism of endocytosis, a fundamental biological process by which cells take up macromolecules and other particles. Many authors have worked on theoretical aspects of membrane mechanics to account for various factors, such as chemical effects and the role of receptors. Of particular interest is the possibility that membrane thinning, or variation of membrane thickness, occurs during deformation and is required for wrapping of extracellular material. We present some recent work on this phenomenon.

Paul Greaney, Martin Meere, Giuseppe Zurlo
National University of Ireland, Galway
paul.greaney@nuigalway.ie,   martin.meere@nuigalway.ie,
giuseppe.zurlo@nuigalway.ie

CP10

Modeling Impact in a Damped 1-D Continuum

We consider the motion of an elastic rod dropped on a fixed foundation subject to gravity and viscous and/or structural damping. The resulting PDE is a Signorini problem. In the case of viscous damping we obtain explicit solution formulas that allow for a precise analysis of the coefficient of restitution (COR) for the impact. In the case of structural damping we rely on a Fourier series approach which allows for convergent numerical investigation of the COR.

Scott Hansen
Iowa State University
Department of Mathematics
shansen@iastate.edu

Feifei Wang
Iowa State University
agnes218ffwang@gmail.com

CP10

On An Adaptive Finite Element Phase-Field Dynamic Fracture Model: Anti-Plane Shear Crack.

In this talk we describe an efficient finite element treatment of a variational, time-discrete model for dynamic brittle fracture. We start by providing an overview of an existing dynamic fracture model that stems from Griffiths theory and based on the Ambrosio-Tortorelli crack regularization. We propose an efficient numerical scheme based on the bi-linear finite elements. For the temporal discretization of the equations of motion, we use generalized $\alpha-$time integration algorithm, which is implicit and unconditionally stable. To accommodate the crack irreversibility, we use a primal-dual active set strategy, which can be identified as a semi-smooth Newton method. It is well known that to resolve the crack-path accurately, the mesh near the crack needs to be very fine, so it is common to use adaptive meshes. We propose a simple, robust, local mesh-refinement criterion to reduce the computational cost. We show that the phase-field based variational approach and adaptive finite-elements provides an efficient procedure for simulating the complex crack propagation including crack-branching.

Mallikarjunaiah S. Muddamallappa
Department of Mathematics
Texas A&M University
msmuddamallappa@wpi.edu

Christopher Larsen
Worcester Polytechnic Institute
Math Dept
cjlarsen@wpi.edu

Marcus Sarkis
Worcester Polytechnic Institute
Instituto de Matematica Pura e Aplicada (Brazil)
msarkis@wpi.edu

CP10

Boundary Value Problems in the Theory of Elasticity of Materials with a Triple Porosity Structure

The theory of elasticity of materials with a triple poros-

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

Merab Svanadze
Ilia State University
svanadze@gmail.com

CP10
Pattern Formation on the Modeling of Multi-Constituent Inhibitory Systems

Skin pigmentation, animal coats and block copolymers, which can be considered as multi-constituent inhibitory systems, are all around us. Theoretical analysis and numerical simulation of multi-constituent inhibitory systems will be provided here. An inhibitory system is studied as a nonlocal geometric variational problem. The free energy of the system is the sum of two terms: the total size of the interfaces separating the constituents, and a longer ranging interaction energy that inhibits micro-domains from unlimited growth. We establish that in different parameter ranges there are corresponding assemblies of certain patterns that exist as the stationary sets of the free energy functional. Numerically, a diffusive interface model is proposed and many self-assembly processes, which form various patterns, are vividly showed here. Different numerical schemes are compared and a new technique is introduced to be consistent with the Euler-Lagrange equation in the sharp interface model.

Chong Wang
George Washington University
chongwang@gwu.edu

Yanxiang Zhao
Department of Mathematics
George Washington University
yxzhao@email.gwu.edu

Xiaofeng Ren
The George Washington University
Department of Mathematics
ren@gwu.edu

CP10
Transformation Groups and Discrete Structures in Continuum Description of Defective Crystals

Davini description of elasticity and plasticity of defective crystal involves a frame of continuum 'lattice vector' fields (lvf), and dislocation density matrix, capturing the structure constants of the Lie bracket of those vector fields. Those fields together describe kinematics of a defective crystal, allowing for elastic and certain plastic deformations, preserving certain invariants A truncation assumption for the energy functional leads to consider finite dimensional Lie algebras of lvf and corresponding transformation groups. In low spatial dimensions, such groups may be clas-

sified. Discrete crystal structures emerge in such context as discrete subgroups of the corresponding Lie groups. This approach includes the usual crystal lattices as a particular case. I will describe explicit form of lvf and discrete structures for defective crystals with non-constant dislocation density in nilpotent (see our paper http://rdcu.be/nD07), solvable, and simple cases, corresponding to 2d crystals with 3d algebras of lattice vector fields.

Maxim Zyskin
School of Mathematical Sciences, University of Nottingham
maxim.zyskin@nottingham.ac.uk

CP11
Efficient Numerical Ice-Sheet Simulations over Long Time Spans

The full-Stokes models to palaeo-ice sheet simulations have previously been highly impractical due to the requirement on the mesh resolution close to the grounding-line. We propose and implement a new sub-grid method for grounding-line migration in full Stokes equations with equidistant mesh. The beauty of this work is to avoid remeshing when the Grounding-line moves from one steady state to another. A new boundary condition is introduced to accommodate the discontinuity in the physical and numerical model. The method is implemented in Elmer/ICE that solves the full Stokes equation with the finite element method. The convergence of the sub-grid method is examined as the mesh is refining and the results are compared with MISMIP benchmark.

Gong Cheng
Department of Information Technology, Uppsala University
cheng.gong@it.uu.se

Lina von Sydow
Uppsala University
Lina.von.Sydow@it.uu.se

Per Lötstedt
Division of Scientific Computing
Uppsala University
perl@it.uu.se

CP11
Modeling and Simulation of Multicomponent, Multiphase Porous Media Flows Using a New Hybrid Method

We use a hybrid method to solve a system of equations modeling surfactant-polymer flooding in porous media. The model includes the effects of capillary pressure and anisotropic dispersion. This is an extension of our recent work [1]. The numerical method is based on the use of a discontinuous finite element method and the modified method of characteristics. The symmetric and non-symmetric, sparse algebraic systems arising from discretization of the associated nonlinear system of governing equations are solved using a BICGstab iterative method with ultra-low tolerance values. Numerical simulations are performed to study the efficiency of various flooding schemes and the effect of anisotropic dispersion. This work has been possible due to financial support from NPRP grant 08-777-1-141 through Qatar National Research Fund and the U.S. National Science Foundation grant DMS-1522782. [1] P. Daripa, S. Dutta, *Modeling and simulation*

of surfactant-polymer flooding using a new hybrid method,
Journal of Computational Physics, **335**, 249–282 (2017).

Sourav Dutta
Texas A&M University
sdutta@math.tamu.edu

Prabir Daripa
Department of Mathematics
Texas A&M University
daripa@math.tamu.edu

CP11

Fire, Ice, Water and Dirt: A Simple Climate Model. An Adventure in Mathematical Modeling

A simple paleoclimate model was developed as a modeling exercise. The model is a lumped parameter system consisting of an ocean (water), land (dirt), glacier and sea ice (ice) and driven by the sun (fire). In comparison with other such models its uniqueness lies in its relative simplicity yet yielding good results. For nominal values of parameters, the system is very sensitive to small changes in the parameters, yielding equilibrium, steady oscillations and catastrophes such as freezing or boiling oceans. However, stable solutions can be found, especially naturally oscillating solutions. For nominally realistic conditions, natural periods of order 100,000 years are obtained, and chaos ensues if the Milankovitch orbital forcing is applied. The key to getting oscillations is having the effective emissivity decreasing with temperature and, at the same time, the effective ocean albedo decrease with increasing glacier extent. Results of the original model compare favorably to the proxy data for ice mass variation, but not for temperature variation. However, modifications to the effective emissivity and albedo can be made to yield much more realistic results. The primary conclusion is that the opinion of Saltzman (1990) is plausible: that the external Milankovitch orbital forcing is not sufficient to explain the dominant 100,000 year period in the data.

John E. Kroll
Department of Mathematics and Statistics
Old Dominion University
jkroll@odu.edu

CP11

Web-Based Software for Surrogate Modeling and Parameter Estimation of Environmental Models Using Clusters of Distributed Computers

Software from various off-the-shelf components and application programming interfaces (API) was used to assemble a tool for developing surrogate expressions of complex environmental simulation models. The browser-based tool contains interactive web pages for configuring a given surrogate modeling approach and launching training runs of the underlying environmental simulation model on a remote cluster of distributed computers. The tool provides an open-source interface for connecting web clients with a given clusters job scheduler. This presentation introduces the different client- and cluster-side components of the tool and describes how all the different pieces fit together. A 600-parameter groundwater modeling and parameter estimation example is also provided to demonstrate the use of the stack in a geosciences context.

Shawn L. Matott
University at Buffalo
Center for Computational Research
lsmatott@buffalo.edu

Eva Wu
Sentient Science
ewu@sentientscience.com

Ramin Bostanabad
Northwestern University
bostanabad@u.northwestern.edu

CP12

A Model for Cell Migration in Non-Isotropic Fibrin Networks with An Application to Pancreatic Tumor Islets

Cell migration is important for tumor growth, immune response and other biomedical processes. This work presents a cell-based model to describe T-lymphocytes migration in non-isotropic fibrin networks around the vicinity of the T-islet in pancreatic cancer. This migration is determined by the mechanical strain energy density as well as by cytokines-driven chemotaxis. Cell displacement is modelled by solving a large system of ordinary stochastic differential equations where the stochastic parts result from random walk, and in which chemotaxis is modelled by the use of Green's Functions that result from treating cells as point sources that secrete chemokines. The stochastic differential equations are solved by the use of the classical Euler-Maruyama method. In this work, the influence of anisotropic stroma on T-lymphocytes migration in different immune systems is investigated. As far as we know, this model presents the first description of pancreatic cancer development under the influence of orientation of the surrounding collagen. As we expected, the model is able to predict that stromal extracellular matrix impedes the immune response of T-cells through changing direction of their migration. Its obstructive effect increases with the degree of anisotropy. Moreover, the model predicts the unlimited proliferation of carcinoma cells if the immune system is weak, and a state of equilibrium where cancer cells are eliminated if the immune system is sufficiently strong.

Jiao Chen
Delft University of Technology
csy_joyce@hotmail.com

Daphne Weihs
Technion-Israel Institute of Technology
daphnew@technion.ac.il

Fred J. Vermolen
Delft University of Technology
F.J.Vermolen@tudelft.nl

CP12

Tree Hydraulics: from Leaves Transpiration to Trunk Sap Flow and Vice Versa

The ascent of water in trees, from the roots to the leaves, for vertical distances that may reach more than a 100 meters, is a problem that has puzzled plant physiologists for a long time. The observed lag between the water flow rate inside the tree trunk, and the water transpiration flux at the leaves, produced many mathematical models, amongst which are PDE porous media models. Very few papers attempt to analyze these models, and instead most resort

to simulations to explain some observed phenomena, and to use them in practical application. Many of the existing models are 1D models that assume only vertical dependence of the flow, and do not include the radial flow component. In at least one paper, a computational method is given to solve the inverse problem of determining transpiration flux from flow measurements in the trunk, but their method gives only bulk transpiration time variation. We propose a 3D angularly symmetric porous medium model, for water flow inside the tree trunk. Through asymptotic analysis, we derive formulas that connect the water flow inside the trunk, to the transpiration flux at the leaves. Using these formulas, we propose a variational formulation, that tackles the inverse problem of recovering the spatial and temporal components of transpiration, given a few discrete noisy measurements of the water flow inside the trunk. This work is potentially useful in environmental studies and in agriculture.

Bebart Janbek
Department of Mathematics
Simon Fraser University
bjanbek@sfu.ca

John Stockie
Simon Fraser University
john_stockie@sfu.ca

CP12
A Mathematical Model of Zika Virus Spread Including Human-Human Transmission

During the last few years, the prevalence of the Zika virus has increased dramatically. This research is based on a model for the Zika virus transmission that takes into account vector-human and human-human transmission. The primary goals are to study the dynamics of the model and to conduct some sensitivity analysis on the parameters, which may differ in different locales. The population dynamics are examined through a modified SEIR model for humans coupled with an SEI model for mosquitoes, resulting in a nonlinear system of differential equations. Parameter ranges are obtained from multiple sources, including values based on human to human sexually transmitted diseases. The system is then solved and analyzed numerically.

Daniel L. Kern
Florida Gulf Coast University
Department of Mathematics
dkern@fgcu.edu

Kelsea Livingstone
Florida Gulf Coast University
krlivingstone9830@eaglefgcu.edu

CP12
Glucose and Urinary Bladder Smooth Muscle Excitability: Role of ATP-Sensitive Potassium Channels

Urinary incontinence (UI), also known as the involuntary urination due to loss of bladder control has a large impact on quality of life. Detrusor smooth muscle (DSM) excitability is considered as a primary cause of UI. ATP-sensitive K+ (KATP) channels provide a link between cellular metabolism and the electrical activities in excitable cells like cardiac myocytes, pancreatic cells, neurons and smooth muscles. We investigated the effects of raised extracellular glucose on DSM cells excitability due to altered KATP channel properties. A computational model of DSM cell was analyzed to investigate the role of KATP channels in eliciting action potentials (APs). We found that incremental extracellular glucose could attenuate the activities of DSM KATP channels. The effect was concentration dependent and involved mainly in macroscopic conductance, not single-channel conductance. In simulations, high levels of intracellular ATP were used to mimic increased extracellular glucose or reduced conductance of KATP channels, enhanced the firing of APs in DSM cell model. This phenomenon of KATP channel attenuation could be one of the underlying mechanisms of glucose-related hyperexcitability. This model provides an elementary tool to investigate the physiological role of glucose concentration underlying the contractions in DSM cells, which in turn can shed light in the genesis of UI.

Chitaranjan Mahapatra, Rohit Manchanda
Indian Institute of Technology Bombay
cmahapatra97@gmail.com, rmanch@iitb.ac.in

CP12
Modeling Ertapenem: The Impact of Body Mass Index on Distribution of the Antibiotic in the Body

Ertapenem is an antibiotic commonly used to treat a broad spectrum of infections. A physiologically-based pharmacokinetic model was developed to investigate the uptake, distribution, and elimination of ertapenem following a once-a-day, single one gram dose. Parameters in the model that were not available in the literature were estimated using an iterative weighted least squares algorithm with published data for blood concentrations of ertapenem for normal height, normal weight males. Simulations were performed to consider the distribution of the antibiotic in men and women with varying body mass indexes. These results could help to determine how dosing regimens should be altered in the future.

Cammey Cole Manning
Meredith College
ManningC@meredith.edu

Michele Joyner
East Tennessee State University
joynerm@mail.etsu.edu

CP12
Modeling the Mitigation of Mosquito-borne Diseases by Infecting Mosquitoes with Wolbachia Bacteria

We develop and analyze an ordinary differential equation (ODE) model to assess the potential effectiveness of infecting mosquitoes with the Wolbachia bacteria to control the ongoing mosquito-borne epidemics, such as dengue fever, Chikungunya, and Zika. Wolbachia is a natural parasitic microbe that stops the proliferation of the harmful viruses inside the mosquito and reduces the disease transmission. A sustainable release for the maternally transmitted Wolbachia bacteria in a wide mosquito population can be difficult due to the induced fitness change and cytoplasmic incompatibility. Our model captures the complex vertical transmission cycle by including heterosexual transmission, multiple pregnant states for female mosquitoes, and the aquatic-life stage. We derive important dimensionless parameters and observe a critical threshold condition for a successful introduction of Wolbachia endemic: the

infection will only persist if the fraction of the infected mosquitoes passes the threshold. This threshold effect is reflected by a backward bifurcation with three coexisting equilibria of the ODE system: a stable disease-free equilibrium, an unstable intermediate-infection endemic equilibrium and a stable high-infection endemic equilibrium. We perform sensitivity analysis on epidemiological and environmental parameters to determine their relative importance to transmission and prevalence. We also compare the effectiveness of different integrated mitigation strategies.

Zhuolin Qu
Tulane University
zqu1@tulane.edu

Ling Xue
University of Manitoba
ling.xue@umanitoba.ca

James Hyman
Tulane University
mhyman@tulane.edu

CP13
Various Extensions of Original Born-Kramers-Slater Model for ReactionsKinetics Based on Brownian Motion and Fokker-Plank Equation Including 1D, 2D, 3D, and Multi-dimensional Approaches

Different extensions, such as Transition State theory of Eyring-Polanyi-Evans model of the original Born-Kramers-Slater Model for the Velocity of Chemical Reactions are discussed based on Smoluchowski and Fokker-Plank equations with various properties of Brownian motion and including 1- dimensional, 2- dimensional, 3- dimensional, and multi-dimensional models with applications in Neuroscience.

Michael Fundator
Sackler Colloquium, National Academy of Sciences of USA
michaelfundator@gmail.com

CP13
Model Reduction Methods Using Koopman Operators for Data Assimilation

Data assimilation are methods that fuse observational data into model to improve the model forecast. These methods are widely used in several areas of science, including weather forecasting, hurricane forecasting, space weather, and subsurface flow, to name a few. In order to reduce the computational burden of assimilating data into large-scale systems, spectral decomposition methods are used to to define a subspace that reduces the dimension of the problem. In this talk we use a recent decomposition technique based on the Koopman operator and present how it applied to data assimilation methods. We will derive an approximation to the eigenfunctions defined by the Koopman operator that represent the non-linear behavior of a dynamical system and use it for a variational data assimilation method. Examples will be presented with simple multi-scale models.

Humberto C. Godinez
Los Alamos National Laboratory
Applied Mathematics and Plasma Physics
hgodinez@lanl.gov

Nicholas Hengartner
Los Alamos National Laboratory
nickh@lanl.gov

CP13
Structure-Preserving Model Reduction for Marginally Stable LTI Systems

This work proposes a structure-preserving model reduction method for marginally stable linear time-invariant (LTI) systems. In contrast to Lyapunov approaches for stable and anti-stable systems, the proposed method can reduce a subsystem with imaginary-axis poles and preserve marginal stability. In particular, the proposed method decomposes a marginally stable LTI system into (1) an asymptotically stable subsystem with eigenvalues in the left-half plane and (2) a marginally stable subsystem with all eigenvalues on the imaginary axis. A new Lyapunov method is proposed to reduce the asymptotically stable subsystem while preserving the inner product structure. In addition, we prove that the marginally stable subsystem with a pure imaginary spectrum is a generalized Hamiltonian system, and as a result, we apply a symplectic method to reduce the marginally stable subsystem while preserving symplectic structure. We formulate a geometric view that unifies the Lyapunov method and the symplectic method for model reduction, and prove that the proposed method preserves the marginal stability of the original system. The stability, accuracy, and efficiency of the proposed technique are illustrated, and compared to existing methods, through two numerical examples.

Liqian Peng
Extreme Scale Data Science & Analytics Department
Sandia National Laboratories
lpeng@sandia.gov

Kevin T. Carlberg, Mohan Sarovar
Sandia National Laboratories
ktcarlb@sandia.gov, mnsarov@sandia.gov

CP13
A Novel Renormalized Mori-Zwanzig Method for Model Reduction

Numerical and analytical simulation methods that capitalize on multiscale structures, both spatial and temporal, have often been used to reduce the dimensionality of high dimensional systems. The Mori-Zwanzig formalism is the general framework for multiscale methods that incorporates a memory term. In this talk, I present a novel approach for constructing a closed reduced order model by approximating the memory term using a bootstrap renormalization-inspired method. This new approach uses fewer assumptions than other popular models based on the Mori-Zwanzig formalism. This model is applied to Burger's equation and the Korteweg-de Vries equation with small dispersion.

Jacob Price
University of Washington
jrp14@uw.edu

CP13
Hierarchical Coarse-Graining of Operators for Md

The length- and time-scale required for semi-crystalline materials or rare-event-phenomena involving low to medium defect concentrations, respectively, far exceed the

currently computationally accessible within the molecular dynamics paradigm. The problem can be resolved by reducing the number of degrees of freedom (DOFs) while increasing timesteps. The topology and sparsity of the bonding structure is used to derive a hierarchical set of DoFs providing a clear framework for full multiresolution beyond the common two-level representation. We connect the hierarchy with wavelets on operator space and the Koopman modes of the infinitesimal time propagator.

Berend C. Rinderspacher
Army Research Laboratory
berend.c.rinderspacher.civ@mail.mil

Jaydeep Bardhan
Northeastern University
j.bardhan@northeastern.edu

Ahmed E. Ismail
Department of Chemical and Biomedical Engineering
West Virginia University
ahmed.ismail@mail.wvu.edu

CP13
Modeling Adsorption in Functionalized Membranes

The emergence of biopharmaceuticals, and particularly therapeutic proteins, as a leading way to manage chronic diseases in humans has created a need for technologies that deliver purified products efficiently and quickly. Towards this end, there has been a significant amount of research on development of porous membranes used in chromatographic bioseparations. In this presentation, we focus on high-capacity multimodal membranes developed by Husson and colleagues in the Department of Chemical and Biomolecular Engineering at Clemson University. To model the protein chromatography process occurring in these functionalized membranes, we consider the reactive transport problem. We incorporate two different nonlinear adsorption models to account for the binding of the protein to the membranes. We begin by assuming instantaneous adsorption and move to considering non-instantaneous adsorption in order to improve the accuracy of the numerical simulations. We will present results from numerical simulations, comparing results obtained using the different adsorption models. We will also compare results of our algorithm with data obtained from laboratory experiments.

Anastasia B. Wilson
Augusta University
Department of Mathematics
anawilson@augusta.edu

Eleanor Jenkins
Clemson University
lea@clemson.edu

CP13
Model Reduction of Chemical Reaction Networks Using L1-Regularization

Large-scale chemical reaction networks such as those used in the study of combustion often involve hundreds of molecular species engaging in thousands of reactions. Model reduction is thus a desirable goal for both identifying key reactions in the network as well as enabling accelerated simulations. In this talk, we will describe a new data-driven method utilizing L1-regularization for reducing systems of reaction rate equations, which involves minimal parameterization and has polynomial-time complexity. We find that the reduced systems have predictive power both when extrapolated in time and in molecular concentration space. Finally, we connect our method to the broader context of model reduction of nonlinear dynamical systems.

Qian Yang
Stanford University
qianyang@stanford.edu

Carlos Sing-Long
Pontificia Universidad Catolica de Chile
casinglo@uc.cl

Evan Reed
Stanford University
evanreed@stanford.edu

CP14
Design of Experiments-Based Geological Uncertainty Quantification of Co2-Based Gas Assisted Gravity Drainage (GAGD) Process

Unlike the conventional gas injection, the Gas-Assisted Gravity Drainage (GAGD) process results in better sweep efficiency and higher microscopic displacement to recover the bypassed oil in the reservoir. The GAGD process takes advantage of natural reservoir fluids segregation to provide gravity stable oil displacement. It consists of placing a horizontal producer near the bottom of the pay zone and injecting gas through vertical wells. The GAGD process was evaluated considering high-resolution compositional reservoir model that includes 3D lithofacies and petrophysical property distribution. Three quantiles of P10, P50, and P90 were incorporated in reservoir model along with Design of Experiments (DoE) to study the heterogeneity and anisotropy effects on the GAGD process. The parameters are horizontal permeability, anisotropy ratio, Pore compressibility, effective reservoir porosity, aquifer size, in addition to CO_2 injection rate, maximum oil production rate, minimum BHP in horizontal producers, and maximum BHP in injection wells. Experimental Design has led to determine the most dominant factors affecting the GAGD performance. Among all the different property realizations, it was clearly seen that anisotropy ratio has direct impact on the process as the 3D lithofacies modeling included Sand, Shaly Sand, and Shale that impede the vertical fluids movement; however, the immiscible CO_2 injection indicated the insensitivity of the GAGD process to reservoir heterogeneities.

Watheq J. Al-Mudhafar
Louisiana State University
wmoham4@lsu.edu

CP14
Field Scale Modeling of Rate-Limited Sorption in Production Transport Codes

Computational models of contaminant transport are used regularly for designing subsurface environmental remediation systems. In many soils, the contaminant sorbs to the solid matrix in the porous media. As a result, the rate of removal by traditional pump-and-treat flushing is much slower than predicted with equilibrium models. This phenomenon is called rate-limited sorption (RLS) and it is particularly problematic in cases where the contaminant has been in place for a long period of time. Although RLS is

well known in academic literature, production models used for field work have failed to incorporate the effect. As a result, remediation designs and cleanup time projections are often inaccurate. In this project, a well-validated production subsurface transport model is modified with a simple analytical model for layers that incorporates RLS effects with reasonable computational costs. Laboratory-scale results are reviewed and the code is applied to a field-scale project. The site is a long-term (over 25 years) cleanup project that may exhibit RLS effects. The results contrast the potential shortfalls in remediation design by using equilibrium modeling.

David L. Coulliette
Mathematics Department
Asbury University
david.coulliette@asbury.edu

Kenneth Rietz, Andrew Ward
Asbury University
kenneth.rietz@gmail.com, andrew.ward@asbury.edu

CP14

Joint Reconstruction with Parametric Level-Set Full-Waveform Inversion

Seismic imaging investigates Earth structures by generating sound waves and recording them at the surface. Full-waveform inversion is a method that tries to produce a map of subsurface parameters by inverting all the seismic data. This process has convergence problems in the presence of high-velocity structures such as salt bodies, anhydrites, or basalt layers. These often have hydrocarbon reservoirs near their flanks or underneath. To improve convergence, we split the Earth model into two parts: sediment, which consists of smoothly varying rock types, and salt geometries with constant properties, which are represented with a level-set function parametrized by radial basis functions. This splitting approach effectively handles the different regularization strategies for smoothness and jumps. We use an alternating minimization technique together with the Gauss-Newton Hessian to accelerate convergence towards the true model. Tests on a stylized salt geometries embedded in a simple sediment model shows promising results.

Ajinkya Kadu
Mathematical Institute, Utrecht University, The Netherlands
a.a.kadu@uu.nl

Tristan van Leeuwen
Mathematical Institute
Utrecht University
t.vanleeuwen@uu.nl

Wim Mulder
Delft University of Technology, The Netherlands
Shell Global Solutions, The Netherlands
wim.mulder@shell.com

CP14

Seismic Imaging and Correlation Analysis of Statistical Fault Zone Model

Presented work is devoted to building and statistical analysis of seismic images of the fault damage zone. In this study we employ a statistical model of fault zone developed in Uni Research CIPR. This model is based on fault facies description of fault zone structure. The results of analysis of deformation bands distribution sampled at 106 outcrops was used to determine the spatial distribution and petrophysical properties of fault facies. Statistical simulation allows us to sample the statistical ensemble of realizations of facies spatial distribution. The seismic modeling is performed for two sets of realization with different variogram ranges. Afterwards the real and the ideal seismic images are built. The comparative analysis of the statistical characteristics of the original facies model and the corresponding seismic imaging is carried out. The coefficients of cross-correlation between the seismic images and seismic ideal images are estimated. We can conclude that the correlation coefficient between the seismic image and ideal seismic images can be used to determine a correct original facies model when comparing set of realizations of seismic images of statistical model with different values of variogram range. Due to the building of ideal images is much less time consuming the obtained results can be used, for example, for numerical solution of inverse problems.

Dmitriy Kolyukhin
(a) Trofimuk Institute of Petroleum Geology and Geophysics
SB RAS Novosibirsk, Russia; (b) Uni CIRP, Bergen, Norway
KolyukhinDR@ipgg.sbras.ru

Vadim Lisitsa
Institute of Petropeum Geology & Geophysics of SB RAS
Russia
lisitsavv@ipgg.sbras.ru

Maxim Protasov
Trofimuk Institute of Petroleum Geology and Geophysics
SB RAS, Novosibirsk, Russia
protasovmi@ipgg.sbras.ru

Dongfang Qu
(a) Uni Research CIPR, Bergen, Norway
(b) University of Bergen, Norway
qudongfang2012@gmail.com

Vladimir Tcheverda
Inst. of Petroleum Geology and Geophysics SB RAS
Russia
cheverdava@ipgg.sbras.ru

Jan Tveranger
Uni CIPR
jan.tveranger@uni.no

Dmitry Vishnevsky
Trofimuk Institute of Petroleum Geology and Geophysics
SB RAS, Novosibirsk, Russia
vishnevsky@ipgg.sbras.ru

CP14

Modelling and Uncertainty Quantification in Biots Poro-Elasticity with Pulsating and Oscillatory Boundary Conditions

Infiltration of large amounts of fresh water into the shallow subsurface would have great value for battling flooding, underground storage of water and reducing the footprint of construction works. A new method to infiltrate high volumes of fresh water has been discovered recently. We refer to this method as Fast, High Volume Infiltration (FHVI).

To describe this infiltration method, we consider a model for aquifers in which water is injected. The flow of water induces local deformations of the aquifer, which are described by Biot's poro-elastic formalism. Our aim is to investigate whether large injection rates induce an oscillatory or a pulsating force near the injection point and whether induced displacements and deformations increase the amount of water that can be injected into the aquifer. For this purpose, a finite-element method based on Taylor-Hood elements has been developed to solve the poro-elastic equations. The study contains simulations with oscillatory force boundary conditions as well as pressure pulses. The results are studied for various oscillatory modes over time as well as over the length of the boundary. Since the oscillatory modes and parameters like the Young's modulus are unknown, we further present results from uncertainty quantification. Since the resulting saddle point problem needs a considerate numerical methodology in terms of possible spurious oscillations, we will also present a stabilised finite-element method.

Menel Rahrah
Delft University of Technology - Faculty of EEMCS - Delft
Institute of Applied Mathematics - Numerical Analysis group
M.Rahrah@tudelft.nl

Fred J. Vermolen
Delft University of Technology
F.J.Vermolen@tudelft.nl

CP14

Calculation of Seismic Depth Migration Before Summation Based on the Asymptotic Solutions of the Telegraph Equation in Parametric Global Coordinate System

We consider the problem of seismic migration for media with a permanent acoustic stiffness oscillations are described by the Klein-Gordon-Fock. The global beam parametric coordinate system for a medium with constant acoustic stiffness, we obtained an asymptotic solution of the seismic migration problem in the form of a compact integral formula. We carried out the implementation of test calculations. Also with this method is considered the inverse scattering problem for inhomogeneous media with local exponential density changes. It is shown that the numerical solution is very accurate analytical approaches.

Ilya Smirnov
Lomonosov Moscow State University
Faculty of Computational Mathematics and Cybernetics
reference20031@rambler.ru

CP15

Mathematical Modeling of Retinal Hemodynamics and Its Relevance in Glaucoma

Several ocular diseases have been associated with impaired retinal perfusion. In glaucoma, many risk factors contribute to ocular damage, including elevated intraocular pressure, age and genetics. Interestingly, alterations in retinal hemodynamics have also been associated with glaucoma. A better understanding of the factors that contribute to these hemodynamic alterations could lead to improved and more appropriate clinical approaches to manage and hopefully treat glaucoma patients. However the interplay among these factors is complex and not always easy to interpret in a clinical setting. The main objective of this work is to use a lumped parameter mathematical model for the retinal circulation to investigate the complex relationship among intraocular pressure, systemic blood pressure, and the functionality of vascular autoregulation. The results obtained with the model help to clarify the outcomes of clinical studies, and show that the insight provided by mathematical modeling alongside clinical studies can improve the understanding of glaucoma and potentially contribute to the clinical development of new treatments.

Simone Cassani
Worcester Polytechnic Institute
scassani@wpi.edu

Giovanna Guidoboni
Indiana University Purdue University Indianapolis
gguidobo@iupui.edu

Julia Arciero
Indiana University-Purdue University Indianapolis
jarciero@iupui.edu

Alon Harris
Indiana University School of Medicine
alharris@indiana.edu

CP15

Evaluating Dosimetric Changes Caused by Positional Errors of the Savi Applicator Used for Breast Cancer Treatment

Breast cancer is the most frequently detected cancer in women in developed countries and is generally diagnosed with women while rarely in men. The research focused on High-Dose-Rate Brachytherapy technique that is an accepted and effective internal radiation to reduce the number of malignant tumor cells. This research investigated the effects of dosimetric changes which are depend upon geometric positioning errors of the radiation source dwell positions. This technique is done by implanting a SAVI applicator to daily deliver a prescribed dose twice for five days. Prior to each administration of the radiation, the SAVI implanted device is inspected to ensure that there is no change such as rotational or translational offset. Source positional errors can typically cause enormous positional changes of the radiation source inside the SAVI catheters which can result in an inaccurate radiation dose. Usually, the inspection of applicator insertion is achieved by CT scan or other imaging devices. It falls into the clinicians and staffs to determine if the changes are clinically significant enough to warrant re-planning the radiation treatment. These changes were compared with previous patients data. Dose Volume Histogram (DVH) has been used to extract the results and evaluate the delivered doses in different organs close to breast tissues. According to the NASBP PROTOCOL B-39, the maximum dose of skin, chest wall, PTV EAVL for V90, V100, V150 and V200 will be evaluated.

Abbas M. Jammali
Ball State University
abbas.mo74@yahoo.com

Andrew Bergan
Ball Memorial Hospital

abergan@iuhealth.org

CP15

On the Computation of Point Spread Functions for the Eye after Contact Lens Motion with Application

A contact lens typically assumes different positions with respect to the pupil after each blink and saccade, and the lens motion may cause a loss in visual acuity. An exact understanding of the loss of acuity is lacking in current literature. Motion of the contact lens can cause significant higher order aberrations (HOA) for myopic patients leading to degradation of visual correction. We estimate the precise 3D lens motion of the lens on the cornea using markers along with an accurate lens model. We compute the change in the point spread function (PSF) of the eye-tear-lens system after lens motion using reverse and forward ray-tracing. The novelty of this work is in the precise computation of the PSF without approximation as we take into account an exact model of the contact lens. This work is of value to optometrists who wish to evaluate contact lens designs. For instance, it is known to optometrists that a lens designed for sphere and cylinder correction may also mitigate some of the HOA caused by lens motion, if some prism is added to the lens in essence, one side of the lens is made thicker in a graded manner in order to minimize rotations on the cornea. We test and validate this hypothesis by computing the retinal images created by lenses with and without added prism using the point spread functions (PSF).

Sanjeewa S. Karunarathna
Texas Tech University
sanjeewa.karunarathna@ttu.edu

Ram V. Iyer
Dept. of Mathematics and Statistics
Texas Tech University
ram.iyer@ttu.edu

Steven Mathews
West Texas Eye Associates
78th street, TX 79424, USA
stevenmmathews@gmail.com

CP15

Activity Patterns in Lateral-Inhibition Type Neural Fields with Asymmetric Excitatory Distal Components

In continuum neural fields, the properties of the connectivity kernel play an essential role in determining the types of observable activity patterns. Amari first demonstrated the existence of stationary bumps for a symmetric lateral-inhibition or Mexican hat type network. Zhang and Guo later showed that an asymmetric coupling function obtained by shifting the Mexican hat in one direction supports traveling pulses. To model distal connections, which are presumed to be excitatory, we augment the Mexican hat kernel by adding to it a purely excitatory shifted hat component. We identify regions in the parameter space which support the existence of traveling pulses and seek corresponding conditions on the relationships among the kernel parameters.

Alex Onderdonk, Myles Akin, Yixin Guo
Drexel University

alexonderdonk100@gmail.com, mga28@drexel.edu, yixinguo@gmail.com

CP15

Establishing a Theoretical Framework for the Ultradian Forced Desynchrony Protocol

In humans, light and other environmental cues entrain a molecular clock with an intrinsic period of approximately 24 h to the exactly 24 h day to maintain internal timekeeping. In order to reliably estimate the intrinsic period of the clock, investigators have developed forced desynchrony (FD) protocols in which participants are exposed to cycles of light and dark with periods outside the range of entrainment of the intrinsic circadian clock. Ultradian FD protocols, in which light/dark cycle periods are 4-5 h, require less time in the lab and are cost effective compared to more common extended day FD protocols, but the effects of protocol design on estimated intrinsic periods have not been established. Using a mathematical model of the circadian pacemaker, we simulated ultradian FD protocols with varying periods, light levels, and study lengths. Since the intrinsic period of the model pacemaker is known, deviations between observed and actual periods under different protocol conditions can be quantified precisely. This analysis establishes a theoretical framework that may be used to optimize the design of ultradian FD protocols to address specific research questions that require an accurate assessment of intrinsic circadian period.

Nora Stack
Department of Applied Mathematics and Statistics
Colorado School of Mines
nstack@mymail.mines.edu

Mary Carskadon
Brown University
University of South Australia
mary_carskadon@brown.edu

David Barker
Brown University
david_barker@brown.edu

Cecilia Diniz Behn
Colorado School of Mines
Applied Math & Statistics
cdinizbe@mines.edu

CP15

On a Diffusion Based Model for Parkinsonian Tremors

The goal is to build a model of Parkinsonian tremors as interactions between the STN and GPE - two regions in the midbrain; the former region excites and the latter inhibits. Tremors are said to occur when the STN neurons have some from of neuronal synchronization. The closest related work in neuronal synchronization is due to DeVille, Peskin and Spencer (2010) but their approach is based on mean-fields and does not take into account inhibition. In current work we start with an discrete markov chain model, take a limit to the continuum, obtain a diffusion and thus a set of PDEs (our model), and then derive various qualitative relationships from the resulting continuous model. No extra assumptions (except for some smoothness assumptions) are made, once the initial markov chain is specified, everything else follows from the initial specifications. Al-

though the model considered is relatively simple, so that we work with 3D diffusions (the 1D case is far less interesting), the important point here is that it allows us to start by specifying the interaction between neurons via a handful of rules, and then extract a continuous time model of neuronal synchronization from it.

Pratik Worah
Google Research
pworah@uchicago.edu

CP16
On the Periodic Doubling and Neimark-Sacker Bifurcations in a Discrete Larch Budmoth Model

The population of the larch budmoth(LBM) in the Swiss Alps is well known for its periodic outbreaks and is one of the best examples of complex population systems. In this study, we investigate a discrete-time leaf quality-LBM population model, where the effect of leaf quality is through budmoths carrying capacity. It is shown that the moth population can persist for all biologically feasible parameter values. Although the LBM can persist indefinitely, we wish to understand whether the population exhibits cyclic dynamics. We establish stability of the moth population when its intrinsic growth rate is small. We derive conditions for period-doubling bifurcations in terms of the intrinsic growth rate of the consumer population when the leaf qualitys recover rate is small. Therefore, the LBM population is more likely to exhibit cyclic behavior if the leaf quality takes a longer time to recover and the LBMs growth rate is larger. Moreover, the system undergoes a Neimark-Sacker bifurcation that produces an invariant closed curve. Numerical simulations are performed to illustrate the bifurcations and dynamics.

Mihiri M. De Silva, Sophia Jang
Texas Tech University
mihiri.de-silva@ttu.edu, sophia.jang@ttu.edu

CP16
Least Action Methods and Noise Induced Transitions in Periodically Forced Systems

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.

John Gemmer
Wake Forest University
Department of Mathematics and Statistics
gemmerj@wfu.edu

Yuxin Chen
Northwestern University
yuxinchen2018@u.northwestern.edu

Alexandria Volkening
Division of Applied Mathematics
Brown University
alexandria_volkening@brown.edu

Mary Silber
University of Chicago
Dept. of Engineering Sciences and Applied Mathematics
msilber@galton.uchicago.edu

CP16
Symbolic Iterative Solution of Boundary Value Problems

We give an efficient method involving symbolic manipulation, Picard iteration, and auxiliary variables for approximating solutions of boundary value problems. We also show how auxiliary variables can be used to give an efficient and widely applicable method involving symbolic manipulation and Picard iteration for approximating solutions of Volterra integral equations. The output is a sequence of polynomials that converges to the true solution exponentially fast with respect to the supremum norm.

Hamid Semiyari
University of Baltimore
UB
hamid.semiyari@gmail.com

CP16
Practical Issues Concerning Parameter Estimation in Distributed Delay Systems

Past events often affect the current state of many biological, sociological, and physical systems, thus the study of dynamical systems involving delays arises naturally. Often, there is variability in the time at which these events occur, and the system is better modeled by a distributed delay. Commonly, we would like to make inferences about underlying processes given observations of a system. While the theoretical framework for parameter estimation methods in a delay system are established, practical issues are relatively poorly understood. Transforming the (infinite dimensional) delay system to a (finite dimensional) ordinary differential equation system is attractive for several reasons. But in so doing, a gamma distribution is assumed for the variability in the time delayed events. I will discuss conditions under which one may have confidence in characterizing the distribution of a delay via least squares estimation, and illustrate problems and pitfalls often encountered. In each case considered, I compare results with those obtained in an ODE system resulting from using the linear chain trick - addressing practical issues such as accessibility, efficiency, and of course accuracy. I will also outline the exploration of current and future questions that have arisen from these preliminary studies, which nonetheless have direct practical consequences when using data to gain insight into a system with a distributed delay.

Karyn L. Sutton
University of Louisiana
Lafayette
sutton@louisiana.edu

CP16
What Is a Random Smooth Function?

The Chebfun project is about continuous analogues of fa-

miliar discrete objects and their realization in Matlab. In Matlab, `randn(n,1)` delivers an n-vector of independent normal $N(0,1)$ samples. What should the analogous Chebfun command `randnfun` deliver? This talk will present the answer we have implemented to that question with applications to numerical simulations of ODEs with noise. It is an interesting mathematical, scientific, and philosophical question whether noise should be most fruitfully regarded as discrete or continuous.

Nick Trefethen
University of Oxford
trefethen@maths.ox.ac.uk

CP16
Stable Foliations Near a Traveling Front for Reaction Diffusion Systems

We establish the existence of a stable foliation in the vicinity of a traveling front solution for systems of reaction diffusion equations in one space dimension that arise in the study of chemical reactions models and solid fuel combustion. In this way we complement the orbital stability results from earlier papers by A. Ghazaryan, S. Schecter and Y. Latushkin. The essential spectrum of the differential operator obtained by linearization at the front touches the imaginary axis. In spaces with exponential weights, one can shift the spectrum to the left. We study the nonlinear equation on the intersection of the unweighted and weighted spaces. Small translations of the front form a center unstable manifold. For each small translation we prove the existence of a stable manifold containing the translated front and show that the stable manifolds foliate a small ball centered at the front.

Xinyao Yang
Xian Jiaotong Liverpool University
XINYAO.YANG@xjtlu.edu.cn

Yuri Latushkin
Department of Mathematics
University of Missouri-Columbia
latushkiny@missouri.edu

Roland Schnaubelt
Department of Mathematics
Karlsruhe Institute of Technology
schnaubelt@kit.edu

CP17
Breaking the Vicious Limit Cycle: Addiction Relapse-Recovery As a Fast-Slow Dynamical System

Symptoms of addictive disorders often manifest as periodic episodes of sudden relapse followed by a relatively long period of recovery. For certain types of addiction, a relapse is precipitated by a state of hyperthymia wherein cravings supersede cessation efforts. Subsequently, a relapse can induce a state of dysthymia which slowly improves concomitantly with the build-up of cravings. To analyze the underlying mechanisms driving relapse-recovery cycles, we construct a fast-slow dynamical system model of the interaction between an addict's propensity to relapse and their current disposition, i.e., craving and mood. The model captures the dynamics of addiction relapse and recovery phenomenologically by admitting relaxation oscillations and canard solutions, which we prove exist by exploiting timescale separation. We derive predictions of cycle period and amplitude to measure relapse frequency and intensity, respectively. As a parameter identified as being responsive to treatment is varied, the system transitions from a state of periodic relapse-recovery to a relapse-free state through reverse Hopf bifurcation. We calculate the threshold value of the treatment parameter, which corresponds to the equilibrium point passing through the fold of the critical manifold.

Jacob P. Duncan
Saint Mary's College, Notre Dame
jduncan@saintmarys.edu

CP17
Pixel Arrays: A Fast and Elementary Method for Solving Nonlinear Systems

We present a new method, called the Pixel Array method, for approximating all solutions in a bounding box, for an arbitrary nonlinear system of relations. In contrast with other solvers, our approach requires the user must specify which variables are to be exposed, and which are to be left latent. The entire solution set is then obtained—in terms of these exposed variables—by performing a series of array multiplications on the n_i-dimensional plots of the individual relations R_i. This procedure introduces no false negatives and is much faster than Newton-based solvers. The key is the unexposed variables, which Newton methods can make no use of. In fact, we found that with even a single unexposed variable our system was more than 10x faster than Julia's NLsolve. The basic idea of the pixel array method is quite elementary, and the purpose of this article is to give a complete account of it.

David I. Spivak, Magdalen Dobson, Sapna Kumari
MIT
dspivak@mit.edu, dobsonm@mit.edu, skumari@mit.edu

CP17
Non Smooth Bifurcation Analysis in a National Electricity Market Model and Its Realistic Approach

This paper proposes a model for the supply and demand of electricity in a domestic market based on system dynamics. Additionally, the model shows piecewise smooth differential equations arising from the diagram of flows and levels, using dynamical systems theory for the study of stability of the equilibrium points that have such a system. A bifurcation analysis approach is proposed in order to define and understand the complex behavior. Until now, no work has been reported related to this topic using bifurcations criteria. The growing interest in personal ways of self-generation using renewable sources can lead the national grid to a standstill and low investment in the system. However, it is important to preserve the national grid as a power supply support to domestic and enterprise demand. In order to understand this scenario, we include an analysis of a zero-rate demand growth. Under this hypothesis, a none smooth bifurcation appears related to a policy which involves the variation of the capacity charge. As a first important result, we found that it is possible to preserve the investments in the market since, through the capacity charge parameter, the system dynamics can be controlled. Then, from a business approach, it is necessary to know the effects of the capacity charge as the strategic policy in the system generation price scheme.

Johnny Valencia
Full Time Professor

Tecnológico de Antioquia - Institución Universitaria
jovalenciacal@unal.edu.co

Gerard Olivar Tost
Department of Mathematics and Statistics
Universidad Nacional de Colombia - Manizales
golivart@unal.edu.co

Carlos Jaime Franco Cardona
Professor
Universidad Nacional de Colombia
cjfranco@unal.edu.co

Isaac Dyner
Professor
Universidad de Bogotá Jorge Tadeo Lozano
isaac.dynerr@utadeo.edu.co

CP18

Simplify Generalized Block Anti-Gauss Quadrature Rules

Golub and Meurant have described how pairs of Gauss and Gauss-Radau quadrature rules can be applied to determine inexpensively computable upper and lower bounds for certain matrix functionals. However, there are many matrix functionals for which this approach is not guaranteed to furnish upper and lower bounds. Then it may be possible to determine such bounds by evaluating pairs of Gauss and anti-Gauss rules. Unfortunately, it is difficult to ascertain the values determined by Gauss and anti-Gauss rules bracket the value of the desired functional. Therefore, generalizations of anti-Gauss rules have recently been described, such that pairs of Gauss and generalized anti-Gauss rules may determine upper and lower bounds also when pairs of Gauss and (standard) anti-Gauss rules do not. The present paper discusses extensions of generalized anti-Gauss rules to include matrix functionals associated with measures in the complex plane and matrix-valued matrix functionals.

Hessah F. Alqahtani
Aurora, Ohio, 44202, USA
halqahta@kent.edu

Lothar Reichel
Kent State University
reichel@math.kent.edu

Miroslav S. Pranic
Department of Mathematics and Informatics
university of Banja Luka
pranic77m@yahoo.com

CP18

Low-Communication FFT

As the costs of arithmetic operations decrease more quickly than the costs for communication, inter-node communication is often the most expensive component of large-scale numerical algorithms. Distributed FFTs are based on the split-radix factorization of the Fourier matrix, which performs three global communications that quickly dominate performance. In this work, we have reformulated and redeveloped a factorization of the FFT matrix that results in a block-dense matrix that exhibits $\mathcal{H}^2$-structure, which allows it to be applied approximately in linear time via the Fast Multipole Method (FMM). The FMM-FFT avoids nearly two thirds of the FFTs communication, but requires much more computation. We show that the FMMs can be efficiently evaluated using GEMM, BatchedGEMM, and other (currently custom) Level-3 BLAS operations, allows highly parallel computations that can be overlapped with the small amount of communication, and provides tunable accuracy parameters. We demonstrate that the FMM-FFT improves on the most recent 1D FFTs available in CUFFTXT 8.0, NVIDIA's multi-GPU FFT library. The FMM-FFT achieves 14-15 digits of accuracy, while achieving approximately a 1.3-1.7x speedup on two P100 GPUs and a 2.1-2.3x speedup on eight P100 GPUs. Analyzing the performances with a roofline model validates this performance, shows that implementations are upward of 90% efficient, and also provides guidance for FMM parameters.

Cris Cecka
NVIDIA Corporation
ccecka@nvidia.com

CP18

High Performance Computing for Sensor Data Fusion and Closed Loop Control in 3D Printing

3D printing has recently evolved from a prototyping tool to the production floor [T. Kellner, Worlds First Plant to Print Jet Engine Nozzles in Mass Production, GE Reports]. However, ensuring quality parts remains a challenge due to an open loop printing process. The current workflow starts with part design, then converts the design to static printer code. The part can only be tested after the print process. This workflow does not allow for adaptive design nor defect correction. It is desirable for a workflow to instead allow for real-time defect detection & print correction. Efforts are ongoing to introduce sensors to monitor printing & enable feedback [J.E. Seppala, et. al., Additive Manufacturing 12 (2016) 7176] [P. Sitthi-Amorn, et. al., ACM Transactions on Graphics 34/4 (2015) 129]. This requires high resolution sensors to counter the printers dynamic & noisy measurement environment. For timely feedback, rapid processing of the high volumes of sensor data is a challenge.

We present work on using high performance computing for *in situ* characterization in 3D printing to enable real-time closed loop control. We address real-time data processing & development of parallel computing algorithms for dynamic fusion of data from multiple sensors to enable decision making. The integration of processing tools written in various software languages will be discussed as will the study of system architectures that utilize the capabilities of CPU & GPU programming.

Michelle Pizzo
Old Dominion University
michelle.e.pizzo@nasa.gov

Travis Taylor
University of Alabama
twtaylor@crimson.ua.edu

Wade Hunter
Old Dominion University
whunt003@odu.edu

Godfrey Sauti
NASA Langley Research Center
Research Aerospace Technologist, Materials & Structures
godfrey.sauti-1@nasa.gov

Dana Hammond
NASA Langley Research Center
Research Aerospace Technologist, Data Systems
dana.p.hammond@nasa.gov

CP18

The Partitioned Global Address Space (PGAS) Approach in Scientific Computing: Case Study of a Compute Bound and a Memory Bound Problem

Writing parallel codes with the classical approach of message passing (MPI) is often perceived as a hard task for scientists. The PGAS paradigm tries to simplify code development while still preserving performance on large clusters.
In this talk, we investigate the development effort and the performance of the PGAS language UPC (Unified Parallel C; an extensive of the C programming language) with the focus on two different case studies:
First we look at a classical fluid dynamics code that uses Godunovs method to solve the Euler equations of gas dynamics. In this code, a Riemann problem is solved at each grid point for each time step, which leads to a compute bound problem.
In the second example, we implement a sparse matrix vector multiplication for a highly unstructured grid resulting from a finite volume discretization of a cardiac simulation. We try to summarize the strengths and weaknesses of the language for scientific code developers and provide some information for what problems PGAS can be considered a viable approach.

Martina Prugger
Department of Mathematics,
University of Innsbruck
martina.prugger@uibk.ac.at

Lukas Einkemmer, Alexander Ostermann
University of Innsbruck
lukas.einkemmer@uibk.ac.at,
alexander.ostermann@uibk.ac.at

Jérémie Lagravière, Johannes Langguth
Simula research laboratory
jeremie@simula.no, langguth@simula.no

Xing Cai
Simula Research Laboratory
1325 Lysaker, Norway
xingca@simula.no

CP18

Distributed-Memory Direct Sparse Matrix Solver for Ansys Electronics

Direct sparse matrix solvers play a critical role in numerous scientific and engineering applications, with the advantage of not needing to construct problem-dependent preconditioners and thus being very robust. However, they may require a large amount of memory and long execution time, even challenging for high-end desktops or workstations. We solve these issues by developing a distributed-memory matrix solver running on computer clusters. Modern clusters consist of many multi-core compute nodes, providing sufficient computational resources. Taking advantage of the hierarchy of clusters, our algorithm first distributes tasks among compute nodes using MPI to transfer data among them, and further partitions each task into finer granular-ity for all cores within a node. Applying the multi-frontal approach, several parallelization strategies are exploited in order to maximize performance. Excellent results are achieved in comparison to an open-source state-of-the-art solver MUMPS.

Zhen Wang
ANSYS
toddwz@gmail.com

CP18

A New Numerical Method for Nonsymmetric Linear Systems

The heavy ball GMRES (HBGMRES) method is one of Krylov subspace methods for nonsymmetric linear systems combined with the restarted GMRES and the heavy ball method which is applied in optimization. HBGMRES not only keeps benefit of the restarted GMRES in limiting memory usage and controlling orthogonalization cost, but also is able to cover up the slow convergence problem in restarted GMRES. A new iterative Krylov subspace method will be presented and comparisons with HBGMRES and restarted GMRES will be shown. Numerical tests on real data are presented to demonstrate the effectiveness of the new methods.

Mei Yang
University of Texas at Arlington
mei.yang@mavs.uta.edu

Ren-Cang Li
University of Texas - Arlington
rcli@uta.edu

CP19

Modeling Intervention Policies for Chlamydia Using Stochastic Network Simulations

Chlamydia trachomatis (Ct) is the most commonly reported STI in the United States with an estimated 1.7 million infections per year. According to the United States Add health there is a 4.9% prevalence of Ct among 18-26 years old sexually active individuals. There is a high prevalence of Ct rate among African American (AA) sexually active people aged 15-25 reside in New Orleans , 8% among men and 12% among women. We create and analyze an individual network-based model for the spread of Chlamydia trachomatis, Ct, in New Orleans. Based on partnership distribution, we made a bipartite sexual network for men and women. We Implemented a MCMC stochastic susceptible-infected-susceptible (SIS) Ct transmission model on this network and identified model parameters that agree with the known Ct incidence in New Orleans. We use the model to quantify the effectiveness of different intervention measures: Partner notification strategies, screening and rescreening of various subgroups, and the effect of condom use are compared in the model.

Asma Azizi Boroojeni
Tulane University
soodeh.azizi@gmail.com

James Mac Hyman
tulane university

mhyman@tulane.edu

CP19
Dual Dilemma of Vaccination

Massive vaccination is beneficial on the population level to suppress the overall epidemic prevalence, but in the mean time, the presence of high vaccination level intensifies the selectively pressure favoring the emergence of vaccine-resistant pathogen strains. This gives rise to the notion of "dual dilemma of vaccination.' Here we address this problem with a combination of game theory and an evolutionary epidemiological model. We will show how the population vaccination level may not only be short of the herd immunity threshold but also cause the potential selection for vaccine-resistant strains that compromise the effectiveness of vaccination. We will also discuss these behavior-disease models to other contexts, such as understanding the tragedy of the commons in overuse of antibiotics.

Xingru Chen, Feng Fu
Dartmouth College
Mathematics Department
xingru.chen.gr@dartmouth.edu, fufeng@gmail.com

CP19
Incorporating Experimental Data into Mathematical Models of Transcription of the RRN Operon

In fast-transcribing prokaryotic genes, such as the rrn operon, many RNA polymerases (RNAPs) transcribe the DNA simultaneously. Active elongation of RNAPs is often interrupted by pauses, which has been observed to cause RNAP traffic jams. Some studies indicate that elongation is faster in the presence of multiple RNAPs than elongation by a single polymerase. Several mathematical models are considered including a nonlinear PDE model as well as a stochastic model where torque imposed by RNAP motion on helically twisted DNA and transmitted to the neighboring polymerases may play a central role in the observed cooperative behavior of polymerases. We have incorporated the torque mechanism and simulated models both with and without torque, including the transcriptional pausing in both cases. The underlying stochastic model is an implementation of the common TASEP framework. For the torque mechanism, the DNA strand between two adjacent RNAPs is modelled as an elastic rod. Simulation results indicate the torque mechanism causes shorter pause durations and fewer collisions between RNAPs. Average transcription rates with torque match experimental data better than those using only the TASEP model without torque, but there is still significant uncertainty in some parameters. Output of model simulations is quite sensitive to parameters describing pause durations as a function of the torque, and uncertainty quantification techniques are used to characterize the variability.

Lisa G. Davis
Montana State University
lisa.davis@montana.edu

Tomas Gedeon
Montana State University
Dept of Mathematical Sciences
gedeon@math.montana.edu

Tamra Heberling
XTD Safety & Surety
Los Alamos National Laboratory

theberling@lanl.gov

CP19
Interalgorithmic Consolidation for Pattern Recognition Applied to Melanoma Genomic Data

Melanoma is a highly proliferative, chemo-resistant disease without a durable response in most patients. Of the available therapies, many have targeted the BRAFV600E mutation that results in abnormal MAPK pathway activation which is important for regulating cell proliferation. These drugs have not proved to be successful leading to the question of what other gene expression changes may be important to consider. In this paper we utilize data from the Cancer Cell Line Encyclopedia (CCLE), including 62 samples, to examine features of gene expression (λ19,000) and copy number (λ24,000) in the skin tumor cell lines to assess which genes are most important for distinguishing cell line clusters. In order to combat the curse of dimensionality in this dataset we adopt a feature selection approach aimed at overall knowledge gain on the feature set that integrates a univariate multiclass Fisher ranking method with well-known powerful machine learning techniques. In comparison to other stand-alone feature selection techniques, our proposed approach provides a subset of features that can more reliably distinguish between genomic subtypes of melanoma cell lines when separately applied to a variety of classification techniques. This method allowed us to identify the top 15 genes from the original 19,000 which provided the same clustering. Of these 15 genes, most are known to be linked directly to melanoma prognosis or other cancers.

Brody J. Kutt
Rochester Institute of Technology
bjk4704@rit.edu

Travaughn Bain
Florida Institute of Technology
tbain2013@my.fit.edu

Rachel Burdorf
Colorado College
rachel.burdorf@coloradocollege.edu

Munevver Subasi
Florida Institute of Technology
Department of Mathematical Sciences
msubasi@fit.edu

Lisa Moore
Florida Institute of Technology
lmoore@fit.edu

CP19
Bayesian Uncertainty Quantification of Dynamic Processes in Networks

We will present a Bayesian uncertainty quantification tool that is applicable to many dynamic processes in networks. We use transitional Monte Carlo Markov Chains (TM-CMC) to populate the posterior distribution for the model parameters. The method is highly parallelizable and can be used on computationally complex systems. While formulating the posterior distributions, the TMCMC algorithm finds the evidence for the model conditioned on the measured data. Thus, it is also relevant to Bayesian model selection. The applications we will look at include finding

aneurysms in arterial networks and locating where an outbreak begins in an SIR epidemic network. This work is done jointly with Petros Koumoutsakos, Costas Papadimitriou, and Panagiotis Hadjidoukas.

Karen Larson, Anastasios Matzavinos
Brown University
karen_larson@brown.edu, anastasios_matzavinos@brown.edu

CP19

Using A Mathematical Model with Individual Patient Data to Quantify Differences Between Patients with Diabetic Foot Ulcers

In this work, we quantify differences in healing responses between type-II diabetic patients with foot ulcers. This work builds off of our previous publication (Krishna et al., B Math Biol, 2015), where we formulate a mathematical model to describe healing responses using averaged timecourse data from another study (Muller et al., Diabet Med, 2008). In Mullers work, they collect data from 16 patients with type-II diabetes. In addition to recording wound areas, Muller also measures levels of matrix metalloproteinases and their inhibitors at Weeks 0, 1, 2, 4, 8, and 12, collected from wound fluid. The patients are divided into two groups categorized as "good healers" and "poor healers" dependent upon the healing response at the four-week point. In our previous work, we use the average data to calibrate our mathematical model and quantify differences between the two groups. In our current work, we have calibrated our mathematical model for each individual patient and have quantified differences between these patients. Also, we are using mixed-effects modeling to further identify differences across patients. Mixed-effects modeling uses both fixed effects, those that do not change across patients, and random effects, those that do change across patients; we are interested in identifying the random effects. In this presentation, we will discuss how our model has identified differences across patients.

Richard Schugart
Western Kentucky University
richard.schugart@wku.edu

CP20

A New Goal-Oriented A Posteriori Error Estimation for 2D and 3D Saddle Point Problems in hp Adaptive FEM

In this research we introduce a new approach on goal-oriented a posteriori error estimation for an automatic hp-Adaptive Finite Element Method. The presented method is based on the classical dual−weighted algorithm. The proposed goal-oriented error estimation requires the solution of local dual problems on patches. The idea of having local patch problems is to apply Clément and Scott−Zhang type interpolation operators to estimate point values with the finite element polynomials. The reliability and also the efficiency of the proposed a posteriori error estimator which are the upper and the lower bounds of the functional error, have been proved. Moreover, the performance of the proposed goal-oriented a posteriori estimator for both $h−$ and $hp−$adaptive FEM has been investigated in numerical examples for Saddle point problem.

Arezou Ghesmati
Texas A&M University
aghesmati@math.tamu.edu

Wolfgang Bangerth
Colorado State University
Texas A&M University
bangerth@colostate.edu

CP20

Parallel Implementation of Finite Element Method with Hexahedral Elements for Forward Modelling of Gravity Data

Finite element method is often employed to solve the forward modelling problem for the inversion of gravity data, as an alternative to forward solvers based on analytic formulas, which usually require lots of computational resources. The inherent sparsity of finite element methods alleviates the minimization costs by solving the resulted linear system with iterative methods which are more memory-efficient. In this paper, a linear finite element method on the basis of hexahedral elements is applied for the forward modelling of gravity data on a domain with topography. Adaptive mesh refinement based on p4est [Carsten Burstedde, Lucas C. Wilcox and Omar Ghattas, p4est: Scalable Algorithms for Parallel Adaptive Mesh Refinement on Forests of Octrees] is employed to obtain a suitable initial mesh, since topographic data is included in the computational domain, and to modify certain regions of mesh locally step by step to result in a better balance between accuracy and requirement of computational resources. In contrast to tetrahedral mesh, the mesh for current finite element method is non-conformal because of the existence of hanging nodes, where continuity of shape functions cannot be retained, hence interpolation is exploited to keep the continuity on hanging nodes. An a posteriori error estimator is used to assess simulation error and determine where mesh refinement is needed. Numerical examples are included to validate the method.

Zhi Li, Lutz Gross
The University of Queensland
z.li2@uq.edu.au, l.gross@uq.edu.au

CP20

A Low-Rank Multigrid Method for the Stochastic Steady-State Diffusion Problem

We study a multigrid method for solving large linear systems of equations with tensor product structure. Such systems are obtained from stochastic finite element discretization of stochastic partial differential equations such as the steady-state diffusion problem with random coefficients. When the variance in the problem is not too large, the solution can be well approximated by a low-rank object. In the proposed multigrid algorithm, the matrix iterates are truncated to low rank to reduce memory requirements and computational effort. The method is proved convergent with an analytic error bound. Numerical experiments show its effectiveness in solving the Galerkin systems compared to the original multigrid solver, especially when the number of degrees of freedom associated with the spatial discretization is large.

Howard C. Elman, Tengfei Su
University of Maryland, College Park
elman@cs.umd.edu, tengfesu@math.umd.edu

CP20

The Entropy and L_2 Stability of Discontinuous Galerkin Methods for the Compressible Euler

Equations

The objective of this presentation is to characterize the entropy and L_2 stability of several representative discontinuous Galerkin (DG) methods for solving the compressible Euler equations. Towards this end, three DG methods are constructed: one DG method with entropy variables as its unknowns, and two DG methods with conservative variables as their unknowns. These methods are employed in order to discretize the compressible Euler equations in space. Thereafter, the resulting semi-discrete formulations are analyzed, and the entropy and L_2 stability characteristics are evaluated. It is shown that the semi-discrete formulation of the DG method with entropy variables is entropy and L_2 stable. Furthermore, it is shown that the semi-discrete formulations of the DG methods with conservative variables are only guaranteed to be entropy and L_2 stable under the assumption that entropy projection errors vanish.

David Williams
Department of Aeronautics and Astronautics
Stanford University
dmw72@psu.edu

CP21
Estimates of Matrix Functions Based on the Lanczos Decomposition

We are concerned with methods for inexpensive approximation of matrix functions f(A)v, where A is a large symmetric matrix, f is a function, and v is a unit vector. It is well known that f(A)v can be approximated by first applying a few steps of the Lanczos process to A with initial vector v, and then evaluating f(T), where T is the small symmetric tridiagonal matrices produced by the Lanczos process. We describe techniques for increasing the accuracy essentially for free and for computing error estimates.

Nasim Eshghi
Kent, Ohio, 44240, USA
Neshghi@kent.edu

Lothar Reichel
Kent State University
reichel@math.kent.edu

CP21
A Two Stage k-Monotone B-Spline Regression Estimator: Uniform Lipschitz Property and Optimal Convergence Rate

With a plethora of applications in science and engineering, constrained estimation garners increasing attention in the areas of applied mathematics and statistics. In particular, k-monotone estimation encompasses a wide range of popular constrained estimation problems, including monotone and convex estimation. In this talk, we consider the asymptotic performance analysis of a novel two stage k-monotone B-spline estimator over a suitable Hölder class for general k. In the first stage, an unconstrained estimator with optimal asymptotic performance is considered; in the second stage, a k-monotone B-spline estimator is constructed by projecting the unconstrained estimator onto a cone of k-monotone splines. To study the asymptotic performance of the second stage estimator, a critical uniform Lipschitz property for the k-monotone B-spline estimator is developed using techniques from spline theory and optimiza-

tion. This result is then exploited to analyze the second stage estimator performance and develop convergence rates under both the sup-norm and mean squared risks. By employing recent results in k-monotone estimation minimax lower bound theory, we show that these convergence rates are optimal.

Teresa Lebair
Johns Hopkins University
tlebair1@jhu.edu

Jinglai Shen
University of Maryland Baltimore County
shenj@umbc.edu

CP21
Fast and Backward Stable Transforms between Spherical Harmonic Expansions and Bivariate Fourier Series

A rapid transformation is derived between spherical harmonic expansions and their analogues in a bivariate Fourier series. The change of basis is described in two steps: firstly, expansions in normalized associated Legendre functions of all orders are converted to those of order zero and one; then, these intermediate expressions are re-expanded in trigonometric form. The first step proceeds with a butterfly factorization of the well-conditioned matrices of connection coefficients. The second step proceeds with fast orthogonal polynomial transforms via hierarchically off-diagonal low-rank matrix decompositions. Total pre-computation requires at best $\mathcal{O}(n^3 \log n)$ flops; and, asymptotically optimal execution time of $\mathcal{O}(n^2 \log^2 n)$ is rigorously proved via connection to Fourier integral operators.

Richard M. Slevinsky
Mathematical Institute
University of Oxford
richard.slevinsky@umanitoba.ca

CP22
Optimization with Invariance Constraints

We introduce a new class of optimization problems which have constraints imposed by trajectories of a dynamical systems. As a concrete example, we consider the problem of optimizing a linear function over a subset of a convex set which remains invariant under the action of a linear, or a switched linear, dynamical system. We identify interesting settings where this problem can be solved in polynomial time by linear programming, or approximated in polynomial time by semidefinite programming.

Amir Ali Ahmadi, Amir Ali Ahmadi
Princeton University
a_a_a@princeton.edu, a_a_a@princeton.edu

Oktay Gunluk
IBM, Watson, New York
gunluk@us.ibm.com

CP22
Time-Varying Convex Optimization

We study linear, quadratic, second order cone, and semidefinite programs whose data (e.g., the matrices A, b, c in the LP case) are not constant but vary polynomially with time. We show that we can approximate the optimal value of

these problems arbitrarily well by searching for solutions that are polynomial functions of time themselves. Furthermore, we show that the problem of finding the optimal polynomial solution of a given degree can be cast exactly as a semidefinite program.

Bachir El Khadir, Amir Ali Ahmadi, Amir Ali Ahmadi
Princeton University
bkhadir@exchange.princeton.edu, a_a_a@princeton.edu, a_a_a@princeton.edu

CP22

Semidefinite Programming for Nash Equilibria in Bimatrix Games

We explore the problem of finding an additive ϵ-approximate Nash equilibrium for bimatrix games with the use of a series of semidefinite programming (SDP) relaxations. We introduce an SDP relaxation for a quadratic programming formulation of the Nash equilibrium (NE) problem. A number of valid inequalities are introduced to improve the quality of this semidefinite relaxation. As usual if a rank-1 solution to the SDP is found, then an exact NE can be recovered. We show that for (generalized) zero-sum games our SDP is guaranteed to have a rank-1 solution. Furthermore, we prove that if a rank-2 solution is found, then a $\frac{5}{11}$-NE can be recovered for a general game, or a $\frac{1}{3}$-NE for a symmetric game. We introduce algorithms based on iterative linearization procedures designed to lower the rank. Empirically, we show that these algorithms often recover rank-2 solutions. Finally, we present a sequence of SDPs based on the Lasserre/sum of squares hierarchy which address NP-hard quantities associated with Nash equilibria.

Jeffrey Zhang, Amir Ali Ahmadi, Amir Ali Ahmadi
Princeton University
jeffz@princeton.edu, a_a_a@princeton.edu, a_a_a@princeton.edu

CP23

Computing PDEs on the Sphere Using Mesh Adaption by Optimal Transport

The numerical solution of PDEs on the sphere is important for problems in meteorology and climate forecasting. To resolve local features in such PDES (such as travelling fronts or storms) it is useful to have a mesh which adapts to the evolving solution. In this talk I will show how it is possible to generate such a mesh efficiently, flexibly and robustly, by moving mesh points on the surface of the sphere. These points will be relocated by solving a nonlinear moving mesh PDE of Monge-Ampere type related to an optimal transport condition. I will show both how this mesh PDE can be solved to give a mesh and will also demonstrate that the resulting meshes can be used effectively in the solution of a variety of different PDEs of interest to meteorological calculations.

Chris Budd
Dept. of Mathematical Sciences
University of Bath, UK
mascjb@bath.ac.uk

Andrew McRae
Department of Mathematical Sciences
University of Bath

a.t.t.mcrae@bath.ac.uk

CP23

Hierarchical Ensemble Kalman Inversion

Since the development of the ensemble Kalman filter (EnKF) it has seen wide extensions from control theory to fields such as data assimilation and inverse problems. This has motivated a recent algorithm which has been used to analyze Bayesian inverse problems in an iterative sense, the iterative EnKF method. This can be viewed as both derivative free and noise controlled. We present an enhancement on this which showcases potential not only to reconstruct the truth, based on a Gaussian form, but also hyperparameters associated with it such as the length scale and the regularity. Numerical results are presented for the Darcy-flow equation and impedance tomography.

Neil Chada
University of Warwick
n.chada@warwick.ac.uk

Andrew Stuart
Computing + Mathematical Sciences
California Institute of Technology
astuart@caltech.edu

Marco Iglesias
University of Nottingham
marco.iglesias@nottingham.ac.uk

Lassi Roininen
Imperial College London
l.roininen@imperial.ac.uk

CP23

Poro-Visco-Elastic Compaction in a Sedimentary Basin

The porosity of a visco-elastic medium is shown to satisfy a nonlinear pseudo-parabolic partial differential equation of the form

$$u' + A(u)\left(\alpha(u) + \eta u'\right) = G(t, u)$$

in which u' denotes the time derivative, $A(v) = -\nabla \cdot \kappa(v)\nabla$ is a linear second order elliptic operator in divergence form with coefficient depending on a function $v(x)$, $G(t, u)$ is a linear first order operator in u, and $\eta > 0$. The third order nonlinear term $A(u)u'$ distinguishes this equation from the classical porous medium equation. The solvability of an elliptic boundary-value problem for $(I + \eta A(v)) u = f$ for $\eta > 0$ and the continuous dependence of the solution u on the function v is used to establish existence and regularity properties of the solution of the initial-boundary-value problem for the pseudo-parabolic equation. These results are obtained by methods of monotonicity and compactness.

Dwight Holland, Ralph Showalter
Oregon State University
holladwi@math.oregonstate.edu, show@oregonstate.edu

CP23

Numerical Investigations of Pattern Formation in Binary Systems with Inhibitory Long-Range Interaction

In this talk, I investigate pattern formation in a two-phase

system on a two-dimensional manifold by numerically computing the minimizers of a Cahn-Hilliard-like model for micro-phase separation of diblock copolymers. The total energy of the system includes a short-range term - a Landau free energy and a long-range term - the Otha-Kawasaki functional. The shortrange term favors large domains with minimum perimeter and the long-range inhibitory term favors small domains. The balance of these terms leads to minimizers with a variety of patterns, including single droplets, droplet assemblies, stripes, wriggled stripes and combinations thereof. We compare the results of our numerical simulations with known analytical results and discuss the stability of the computed solutions and the role of key parameters in pattern formation. For demonstration purposes, we focus on the triaxial ellipsoid, but our methods are general and can be applied to higher genus surfaces and surfaces with boundaries.

Jiajun Lu
siam member
lujiajunchuguo@126.com

Frank Baginski
George Washington University
baginski@gwu.edu

CP23

A Diffusion Limit For A Finite Capacity Storage Allocation Model

We give some asymptotic results for the following storage allocation model: There are m primary spaces, ranked $\{1, 2, \cdots, m\}$, and R secondary spaces, ranked $\{m+1, m+2, \cdots, m+R\}$. Customers arrive according to a Poisson process with rate parameter λ, a new arrival takes the lowest ranked space, and occupies it for an exponentially distributed amount of time, with mean $1/\mu$. Letting N_1 and N_2 be, respectively, the numbers of occupied primary and secondary spaces, we recently obtained an explicit, albeit complicated, expression for the joint steady-state distribution, $\pi(k, r) = \mathbb{P}[N_1 = k, N_2 = r]$. We also obtained various asymptotic results for this distribution, in the limit where $\rho \equiv \lambda/\mu \to \infty$, but with $m, R = \Theta(\rho)$. Here we consider a different limit, where $\rho \to \infty$ with $m = \rho + O(\sqrt{\rho})$ and $R = O(\sqrt{\rho})$. Then we obtain a limiting two-dimensional density as a leading order approximation to $\pi(k, r)$. We also examine various asymptotic properties of this density, including tail behaviors, and give numerical comparisons to the discrete model. Finally we show that the density satisfies a certain two-dimensional parabolic partial differential equation (PDE) with appropriate boundary/corner conditions.

Eunju Sohn
Columbia College Chicago
esohn@colum.edu

Charles Knessl
University of Illinois at Chicago
knessl@uic.edu

CP24

A Convolutional Network Approach for Image Reconstruction from a Single X-Ray Projection

To treat lung cancer patients, it is important to eliminate blurring artifacts in 3D images reconstructed from a set of 2D x-ray projected data. The motion blur is prominent in the thorax due to breathing. We aim at developing a machine learning algorithm that allows for time-resolved volumetric reconstruction from a single projection image. In our approach, each volumetric image is represented as a deformation of a chosen reference image. We model the deformations as a linear combination of a set of basis deformations through principal component analysis (PCA). Based on the PCA deformation model, we generate training data and train a convolutional neural network (CNN) to find a mapping from a projection image to PCA coefficients. To further improve the efficiency, we pre-process the projection images by taking the gradient, select a small number of patches that contain valuable motion information (e.g., diaphragm region) and train the CNN. When it comes to image reconstruction, we can obtain a volumetric image by applying the mapping on an instantaneous projection image. We validate our method on a set of simulated data. Our CNN model has the flexibility to deal with other artifacts in real data, which will be explored in the future.

Conner S. Davis, Samiha Rouf
University of Texas at Dallas
conner.davis@utdallas.edu, scr091020@utdallas.edu

Yifei Lou
The University of Texas at Dallas
yxl145331@utdallas.edu

Yan Cao
University of Texas at Dallas
yxc069200@utdallas.edu

CP24

Terminating Iterative Regularization Algorithms for Large-Scale Ill-Posed Problems Using the Picard Parameter

Late stopping of iterative regularization of large-scale ill-posed problems results in solutions with a high amount of noise. Unfortunately, state-of-the-art methods are often inconsistent in their estimation of the stopping iteration, giving suboptimal solutions in a significant percentage of problems and noise instances. We explain the reason for this inconsistency and develop a new stopping-criterion which overcomes the shortcomings of the previous methods. The new stopping criterion which approximately minimizes the prediction error, relies on filtering the given noisy data in the basis of the discrete Fourier transform (DFT) using the Picard parameter. The Picard parameter separates the noise-dominated Fourier coefficients of the data from the clean ones in one dimension in the basis of the SVD of the coefficient matrix of the problem. However, we show that it can be extended to the basis of the DFT of the noisy image as well, achieving a similar effect. To use the Picard parameter for two-dimensional problems, we also present a novel vectorization scheme for the 2D DFT of an image. Our stopping criterion is demonstrated to outperform state-of-the-art methods when it is applied to the Golub-Kahan iterative process.

Eitan Levin, Alexander Meltzer
Department of Condensed Matter Physics
Weizmann Institute of Science
eitan.levin@weizmann.ac.il,   alexander.meltzer@weizmann.ac.il

CP24

Simultaneous Corneal Curvature and Elevation Computation from Optical Coherence Tomography

Data

Due to prevalence of refractive surgery, early screening for ectatic diseases of cornea such as Keratoconus is becoming increasingly important in ophthalmology. Two important metrics for disease diagnosis are local power, and shape of the corneal surface. A third metric is the thickness of the corneal surface, which is not addressed in this research. A Placido-disc videokeratographer yields average power of the cornea through axial and tangential curvature maps. A major limitation of these curvature maps is that they are not invariant with respect to change of coordinates. We compute the mean curvature of the cornea in this research, which is invariant with respect to diffeomorphisms. The clinical limitation of curvature maps is that they cannot be used in isolation to diagnose pathologies due to natural variations in corneal shape in the population. Imaging devices such as Slit-scanning topographer, Scheimpflug imager, and optical coherence tomographers (OCT) provide elevation information for the cornea as a sparse 3D cloud of points. This data may be used in a traditional image processing approach to construct a linear spline approximation to the corneal surface. However, a linear spline cannot yield the mean curvature at any point on the corneal surface. We present an algorithm to compute a quartic spline approximation to the corneal surface which simultaneously yields both elevation and mean curvature. Application to data from an OCT will be presented.

Farzana Nasrin
Texas Tech University
Department of Mathematics and Statistics
farzana.nasrin@ttu.edu

Ram V. Iyer
Dept. of Mathematics and Statistics
Texas Tech University
ram.iyer@ttu.edu

Steven Mathews
West Texas Eye Associates
78th street, TX 79424, USA
stevenmmathews@gmail.com

CP24

Detecting Breast Masses and the Location of the Prostate

I will present a fast Enclosure Transform to localize complex objects of interest from speckle imagery. This approach explores spatial constraints on regional features from a sparse image feature representation. Unrelated, broken ridge features surrounding an object are organized collaboratively, giving rise to the enclosureness of the object. Three enclosure likelihood measures are constructed, consisting of the enclosure force, potential energy, and encloser count. In the transform domain, the local maxima manifest the locations of interest objects, for which only the intrinsic dimension is known a priori. I will demonstrate two medical applications in detecting (1) suspicious breast masses in screening breast ultrasound, and (2) the location of the prostate in trans-abdominal ultrasound for verification of patient positioning in radiotherapy treatment of prostate cancer.

Jue Wang
Union College
wangj@union.edu

CP24

Variational Approaches to the Restauration of Manifold-Valued Signals and Images

Manifold valued data appear in various applications in image processing and imaging. Important examples are nonlinear color spaces, the rotation group and the Riemannian symmetric space of positive matrices. In this talk, we present our algorithmic schemes for the TV regularization of manifold-valued data. In particular, we also consider a setup with indirectly measured data. We further present our approaches for Blake-Zisserman and Potts problems which are discrete variants of the Mumford-Shah model and the piecewise constant Mumford-Shah model for manifold-valued data. We show the potential of our algorithms using DTI data. This talk is based on joint work with M. Storath, L. Demaret, M. Baust, M. Wieczorek, T. Lasser, and N. Navab.

Andreas Weinmann
HelmholtzZentrum München
andreas.weinmann@helmholtz-muenchen.de

CP25

Accurate, Stable Boundary Conditions for Downwind-Biased Discretizations of Hyperbolic PDEs

Strong stability preserved (SSP) methods with downwinding (also referred to as perturbed methods) have been introduced at the same time the SSP theory appeared. However, until now perturbed methods have been only used with periodic boundary conditions. In this talk, we provide a rigorous analysis of various boundary conditions applicable to Runge–Kutta methods that use both upwind- and downwind-biased discretizations for hyperbolic conservation laws. In addition, we examine the boundary conditions under which a perturbed Runge–Kutta method coupled with a TVD spatial discretization maintains the TVD property. Several examples in one- and two-dimensional hyperbolic problems exhibit the robustness of the boundary condition treatment and the high order of accuracy at the boundaries.

Yiannis Hadjimichael
King Abdullah University of Science and Technology
(KAUST)
yiannis.hadjimichael@kaust.edu.sa

David I. Ketcheson
King Abdullah University of Science & Technology
(KAUST)
david.ketcheson@kaust.edu.sa

CP25

Radial Basis Function generated Finite Differences for Pricing Multi-Asset Financial Derivatives

Pricing of financial derivatives is a very important task for reliable trading, investment strategy development and calibration of financial models. Many of such contracts are issued on several underlying assets. Consequently, their pricing leads to complex high-dimensional problems, often requiring advanced high-performance numerical treatment in order to be solved. Therefore, a mesh-free and sparse numerical method known as radial basis function generated

finite differences (RBF-FD) is developed as an efficient way to tackle multi-asset options. The method is a mesh-free generalization of classical finite differences, derived as a localized version of radial basis function approximation, and as such is exploiting the best properties from both of the approaches. We present the most recent improvements in RBF-FD methods and its performance results applied in option pricing. The main focus is on the benefits of using polyharmonic splines (PHS) to avoid the shape parameter tuning problems that previous attempts were featured with and applying smoothing of initial conditions to enable proper convergence order.

Slobodan Milovanovic, Lina von Sydow
Uppsala University
slobodan.milovanovic@it.uu.se, Lina.von.Sydow@it.uu.se

CP25
Stability of BDF-ADI Discretizations

We present new results on absolute stability for BDF-ADI (Backward differentiation formula Alternating Direction Implicit) methods applied to hyperbolic, parabolic and mixed PDEs with Fourier spectral collocation in space. Unconditional absolute stability of BDF2-ADI method (order 2) for the hyperbolic case is proven. Moreover, conditional absolute stability of BDF2-ADI to BDF5-ADI is also proven for the parabolic case. The ADI methodology followed is the Douglas-Gunn splitting along with extrapolation of the mixed terms.

Joao Reis
King Abdullah University of Science and Technology
CEMSE Division
joao.feliciodosreis@kaust.edu.sa

David I. Ketcheson
CEMSE Division
King Abdullah University of Science & Technology
david.ketcheson@kaust.edu.sa

Lajos Loczi
King Abdullah University of Science and Technology
CEMSE Division
lajos.loczi@kaust.edu.sa

CP25
The Saddle-Point Method for the Complex Helmholtz Equation

The Helmholtz equation is notoriously difficult to solve using standard iterative methods. This talk presents a new finite element method for the complex Helmholtz equation that relies entirely on solving positive definite systems of equations with Conjugate Gradient and Multigrid. The basis for this method is the saddle-point variational principles of Milton, Seppecher, and Bouchitte. An error bound for the method an numerical examples will be given, including implementation of the algorithm on a GPU.

Russell B. Richins
Thiel College
rrichins@thiel.edu

CP25
On the Numerical Integration of Initial-Boundary Value Problem to One Nonlinear Parabolic Equation

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

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

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

Mikheil Tutberidze
Ilia State University
Associated Professor
mikheil.tutberidze@iliauni.edu.ge

CP25
A Weno Method Based on Exponential Polynomials for Hyperbolic Conservation Laws

The aim of this study is to develop a novel sixth order weighted essentially non-oscillatory (WENO) finite difference scheme. On the purpose of designing new WENO weights, we present two important measurements: discontinuity detector (at the cell boundary) and smoothness indicator. The interpolation method is implemented by using exponential polynomials with tension parameters such that they can be tuned to the characteristics of a given data, yielding better approximation near steep gradients without spurious oscillations than the WENO schemes based on algebraic polynomials at the same computational cost. A detailed analysis is performed to verify that the proposed scheme provides the required convergence order of accuracy. Some numerical experiments are presented and compared with the other sixth-order WENO schemes to demonstrate the new algorithm's ability.

Youngsoo Ha
Department of Mathematics, Seoul National University, Seoul, Republic of Korea
youngamath.ha@gmail.com

Chang Ho Kim
Department of Computer Engineering, Glocal Campus, Konkuk University, Chungju, Republic of Korea
kimchang@kku.ac.kr

Hyoseon Yang
Department of Mathematics, Ewha Womans University, Seoul 03760 Republic of Korea
hyoseon1989@gmail.com

Jungho Yoon
Dept. Mathematics, Ewha W. Univ.,
Seoul, S.Korea
yoon@ewha.ac.kr

CP26
Sufficient Conditions for Logconcavity of Multivariate Discrete Distributions

This project presents sufficient conditions for trivariate discrete distributions to be logconcave. A special subdivision

of R^n is used to obtain a sufficient condition that ensures the logconcavity of multivariate discrete distributions. Examples of logconcave multivariate discrete distributions are presented. A dual type linear programming approach is proposed to maximize logconcave multivariate discrete distributions.

Majed Alharbi
Florida Institute of Technology
malharbi2013@my.fit.edu

Ersoy Subasi
Florida Institute of Technology
Department of Engineering Systems
esubasi@fit.edu

Munevver Subasi
Florida Institute of Technology
Department of Mathematical Sciences
msubasi@fit.edu

CP26
Optimization of Multi-Measuring Systems with Control Parameters and its Application to Polarized Light Microscopy

Today's state-of-the-art of experimental techniques often integrate computers in the experimental setup. Computers serve not only for real-time data analysis, but also control and change measuring conditions. The computer control allows to design experimental setups that determine n characteristics of an explored object from k measurements, performed under different sets of control parameters. In this work we investigate method for determining optimal control parameters of such multi-measuring systems. Our choice is based on perturbation analysis and reduces the sensitivity of measured quantities. As an example, we applied our method for the PolScope, - polarized light microscope, designed to study optical patterns of thin biological and soft matter samples by determining their two-dimensional distributions of retardance magnitude and of slow axis direction. In the PolScope, variable retardances of two liquid-crystal plates are control parameters which modulate polarization states of incident illuminating light. The accuracy of the measurements achieved with our approach is compared to the accuracy obtained with the parameter setting defined by the software provided with the PolScope.

Mykhailo Kuian, Lothar Reichel
Kent State University
mkuian@kent.edu, reichel@math.kent.edu

Shiyanovskii Sergij
Kent State University,
Institute of Liquid crystals
sshiyano@kent.edu

CP26
A Cut-Based Heuristic for Solving the Bi-Directional Single-Row Machine Layout Problem

The optimal assignment of workstations in a bi-directional linear flow layout with fixed input/output stations at opposite ends is to be determined to minimize the total material flow cost. Equivalence of this layout problem and the corresponding network optimization problem has been demonstrated. We also show that the minimization of total flow cost is equivalent to the minimization of total backtracking flow cost in this layout problem. An efficient polynomial time $O(n^4)$ algorithm that is based on the cut approach in the location model is developed and tested to find the optimum or near optimum sequence for equidistant linear layout problem, where n is the number of machines in the layout. The computational study has demonstrated that the proposed heuristic is efficient and effective. The average cost deviation is less than 0.6%, when the approximate solution is compared with that in the optimization model.

Shine-Der Lee, Chuan-Chien Cheng
National Cheng Kung University
Dept. of Industrial & Information Management
sdlee@mail.ncku.edu.tw, believe92317@gmail.com

CP26
Volume Calculations for Sparse Boolean Quadric Relaxations

With the idea of measuring the quality of convex relaxations of non-convex sets, Lee and Morris (1994) introduced the idea of utilizing d-dimensional volume for this purpose. Ko, Lee, and Steingrímmson (1997) got a closed form expression for the volume of a simple polyhedral relaxation of the boolean quadric polytope (BQP) of a complete graph. We extend their result to simple sparse graphs and algorithmically to graphs of bounded tree width. Additionally, we get a formula for the volume of the BQP of a cycle, and some results towards the solution for series-parallel graphs.

Daphne Skipper
United States Naval Academy
skipper@usna.edu

Jon Lee
University of Michigan
jonxlee@umich.edu

CP26
New Bounds for the Probability That at Least K-Out-of-N Events Occur with Unimodal Distributions

The contribution of the shape information of the underlying distribution in probability bounding problem is investigated and a linear programming based bounding methodology to obtain robust and efficiently computable bounds for the probability that at least k-out-of-n events occur is developed. The dual feasible bases structures of the relaxed versions of linear programs involved are fully described. The bounds for the probability that at least k-out-of-n events occur are obtained in the form of formulas as well as the result of customized algorithmic solutions of the linear programs involved. Applications in PERT to estimate the length of critical path, in finance to estimate the European Option Call price, and in reliability to estimate k-out-of-n type system reliability are presented.

Munevver Subasi
Florida Institute of Technology
Department of Mathematical Sciences
msubasi@fit.edu

Ersoy Subasi
Florida Institute of Technology
Department of Engineering Systems
esubasi@fit.edu

Ahmed Binmahfoudh
Florida Institute of Technology
Department of Mathematical Sciences
abinmahf2007@my.fit.edu

Andras Prekopa
Rutgers University
Rutgers Center for Operations Research
prekopa@rutcor.rutgers.edu

CP26
Vehicle Routing Problem with Interdiction

In this paper, we study the role of interdiction in the Vehicle Routing Problem (VRP), which naturally arises in humanitarian logistics and military applications. We assume that in a general network, each arc has a chance to be interdicted. When interdiction happens, the vehicle traveling on this arc is lost, thus unable to continue the trip. We model the occurrence of interdiction as a given probability and consider the multi-period expected delivery. Our objective is to minimize the total travel cost or to maximize the demand fulfillment, depending on the supply quantity. This problem is called the Vehicle Routing Problem with Interdiction (VRPI). We first prove that the proposed VRPI problems are NP-hard. Then we show some key analytical properties pertaining to the optimal solutions of these problems. Most importantly, we examine Dror and Trudeau's property applied to our problem setting. Finally, we present efficient heuristic algorithms to solve these problems and show the effectiveness through numerical studies.

Michael Xu
McMaster University
xum19@mcmaster.ca

CP27
Viscosity Solutions of Stationary Hamilton-Jacobi Equations and Minimizers of L^∞ Functionals

Existence results for viscosity solutions to the Dirichlet problem for stationary Hamilton-Jacobi equations, the associated relaxed problem via quasiconvex envelopes, and for minimizers of the corresponding L^∞ functionals are obtained for given boundary data in $W^{1,\infty}$. Joint work with Nick Barron and Robert Jensen.

Marian Bocea
Loyola University Chicago
mbocea@luc.edu

CP27
Fractional Integrated Semi Groups and Nonlocal Cauchy Problem for Abstract Nonlinear Fractional Differential Equations

Some classes of fractional abstract differential equations with α-integrated semi groups are studied in Banach space. The existence of a unique solution of the nonlocal Cauchy problem is studied. Some properties are given.

Mahmoud M. El-Borai
Professor of Mathematics Faculty of Science Alexandria Unive
Alexandria University Egypt
m_m_elborai@yahoo.com

Khairia E. El-Nadi
Prof of Mathematical Statistics Dep. of Math. Faculty of Science Alexandria University Alexandria Egypt
Khairia_el_said@Hotmail.com

CP27
Asymptotic Analysis of a Drying Model Motivated by Coffee Bean Roasting

Understanding heat, moisture, and mass transport during the roasting of a coffee bean is essential to identifying the colour and flavours of the final product. Recent modelling of coffee bean roasting suggests that in the early stages of roasting, there are two emergent regions: a dried outer region and a saturated interior region. These two regions are separated by a moving transition layer (or drying front). We will consider the asymptotic analysis of this drying process in order to gain a better understanding of its salient features. The model consists of a PDE system governing the moisture and gas pressure profiles throughout the interior of the bean. By obtaining asymptotic expansions for these quantities in relevant limits of the physical parameters, we are able to determine the qualitative behaviour of the outer and interior regions, as well as the dynamics of the drying front. Indeed, we find that for all of the asymptotic limits considered, our approximate solutions faithfully reproduce the qualitative features evident from numerical simulations.

Nabil T. Fadai, Colin Please, Robert Van Gorder
University of Oxford
nabil.fadai@maths.ox.ac.uk, colin.please@maths.ox.ac.uk,
robert.vangorder@maths.ox.ac.uk

CP27
Stochastic Simulation of Reaction-Diffusion Systems: Fluctuating Hydrodynamic Approach

We develop numerical methods for reaction-diffusion systems based on the equations of fluctuating hydrodynamics (FHD). While the FHD formulation is formally described by stochastic partial differential equations (SPDEs), it becomes similar to the reaction-diffusion master equation (RDME) description when those SPDEs are spatially discretized and reactions are modeled as a source term having Poisson fluctuations. However, unlike the RDME, the FHD description naturally extends from the regime where fluctuations are strong, i.e., each hydrodynamic cell has few (reactive) molecules, to regimes with moderate or weak fluctuations, and ultimately to the deterministic limit. By treating diffusion implicitly, we avoid the severe restriction on time step size that limits all methods based on explicit treatments of diffusion, and construct numerical methods that are more efficient than RDME methods, without compromising accuracy. We construct several two-stage (predictor-corrector) schemes, where diffusion is treated using a stochastic Crank–Nicolson method, and reactions are handled by the stochastic simulation algorithm of Gillespie or a weakly second-order tau leaping method. We present simulation results for a two-dimensional Turing-like pattern formation and a three-dimensional chemical front propagation. We also discuss the inclusion of stochastic reactions to the full FHD equations.

Changho Kim, Andy Nonaka
Lawrence Berkeley National Laboratory
changhokim@lbl.gov, ajnonaka@lbl.gov

John B. Bell

CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

Alejandro Garcia
San Jose State University
alejandro.garcia@sjsu.edu

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

CP27

Process of Optimization of Free Parameters in Stabilized Methods

Stabilized methods for convection-dominated problems require the choice of appropriate stabilization parameters in SUPG (SDFEM) or SOLD (spurious oscillations at layers diminishing) methods. From numerical analysis only bounds on these free parameters are known. We will present how such an optimization process regarding stabilization parameters looks like in the detail. We minimize a target functional which is a residual-based error indicator. Benefits of the basic approach are demonstrated by means of numerical results. The optimization process and it's specifics will be carefully presented.

Petr Lukas
Charles University
lukas@karlin.mff.cuni.cz

CP27

Large Deviations for a Stochastic Korteweg-De Vries Equation with Additive Noise

We prove the large deviation principle for the law of the solutions to a stochastic Korteweg-de Vries equation in the presence of an additive noise. Our proof is based on the weak convergence approach.

Leila Setayeshgar
Providence College
lsetayes@providence.edu

Chia Ying Lee
University of British Columbia
U. of North Carolina
lchiaying.lee@gmail.com

CP27

A Novel Deformation Method for Higher Order Mesh Generation

In [G.Liao et.al, Adaptive Grid Generation based on the Least Square Finite Element Method(LSFEM)], the prescribed positive Jacobian determinant is essential and a LSFEM had built to solve the Div-Curl system that appears in Liao's mesh deformation method for grid generation. In this work, similarly to [G.Liao et.al, New Techniques for Grid Generation and Adatptation], This method is extended to generate higher order mesh by an adaptive moving mesh technique. Numerical examples for p=3 will be shown to demonstrate the procedures and its effectiveness. This method will be compared to some other approaches based on preservation of positive Jacobian determinant. The applications in image registration will also be discussed, as presented in [G.Liao et.al, New Development of Nonrigid Registration], [X.Chen et.al, New Variational Method of Grid Generation with prescribed Jacobian determinant and prescribed curl] and [X.Chen et.al, New method of averaging diffiomorphisms based on Jacobian determinant and curl vector].

Guojun Liao
Department of Mathematics
University of Texas at Arlington
liao@uta.edu

Zicong Zhou
University of Texas at Arlington
zicong.zhou@uta.edu

CP28

On Jacobi Methods for the Positive Definite Generalized Eigenvalue Problem

We derive and consider several new Jacobi methods for the positive definite generalized eigenvalue problem $Ax = \lambda Bx$, where A is symmetric and B is symmetric positive definite matrix. They are based on LL^T, RR^T and the spectral decomposition of the pivot submatrix of B. A hybrid method, which combines all three methods, and a general Jacobi method for PGEP are also considered. Connection with the Falk-Langemeyer method has been analyzed. The global convergence of all those methods is proved under the large class of generalized serial strategies. High relative accuracy and asymptotic convergence have also been investigated. A hybrid method can be much more accurate than its component methods. Special attention is paid to the case of multiple eigenvalues of the problem. All these element-wise methods can serve as kernel algorithms for the associated block Jacobi methods which are suitable for CPU and GPU computing. When implemented as one-sided block methods for the generalized singular value problem, they are very efficient, and highly accurate on well behaved matrices. The global convergence of the block methods has also been considered.

Vjeran Hari
University of Zagreb
hari@math.hr

CP28

The Vector Space of Finite Summations and Its Applications

In this lecture we present algebraic properties of the vector space of matrices generated by partial sums of vectors in $\mathbb{R}^n$. Vector space of finite summations is related to Fourier transforms and to certain discrete stochastic processes, and to the one dimensional Poisson equation. As an application, we provide a new method for noise reduction in signal processing based on a variance weighted Fourier sine transform. We present two numerical examples to demonstrate the behavior of the cumulative power spectral density (CPSD) algorithm. The first example contrasts our algorithm with the standard Savitsky-Golay algorithm, which is widely used in spectroscopy. The second example demonstrates its behavior on one instance of real Raman spectra. The algorithm automatically acts as an extreme low pass filter. In the outcome, almost all high energy and high frequency "noise' are automatically discarded.

Pawel B. Marcinek
Oakland University

Department of Mathematics and Statistics
pbmarcin@oakland.edu

Peter Shi
Oakland University
pshi@oakland.edu

Serge Kruk
Department of Mathematics and Statistics
Oakland University, Rochester, MI
kruk@oakland.edu

CP28

Robust Linear Stability Analysis and a New Method for Computing the Action of the Matrix Exponential

Linear stability analysis of a large-scale dynamical system requires computing the rightmost eigenvalue of a large, sparse matrix A. To enhance the convergence of this eigenvalue, an iterative eigenvalue solver is frequently applied to a transformation of A instead, which plays a similar role as a preconditioner for linear systems. Commonly used transformations such as shift-invert are unreliable and may cause the convergence to a wrong eigenvalue. We propose using the exponential transformation since the rightmost eigenvalue of A corresponds to the largest eigenvalue of e^A, which is preferred by iterative eigenvalue solvers. Several challenging eigenvalue problems that stem from both linear stability analysis and pseudospectral analysis demonstrate the robustness of the exponential transformation at 'preconditioning' the rightmost eigenvalue. The key to the efficiency of this preconditioner is a fast algorithm for multiplying e^A and a vector. We develop a new method based on a rational approximation of e^x with only one (repeating) pole. Compared to a polynomial based method, it is observed to converge much more rapidly when the spectrum of A has a wide horizontal span, which is common for matrices arising from PDEs.

Minghao W. Rostami
Syracuse University
mwrostam@syr.edu

Fei Xue
Clemson University
fxue@clemson.edu

CP28

A Nonlinear Krylov-Type Method for Differentiable Mixed Subordinate Matrix Norms

We propose a new method for approximating a mixed subordinate matrix norm $\|A\|_{\beta \to \alpha}$ defined by any two Gâteaux differentiable vector norms. The underlying idea is to accelerate the popular nonlinear power method by building at each step an approximation on the subspace spanned by the previous approximations. This is reminiscent of the Krylov subspace method for matrix eigenvalues, in which case the subspace optimization step can be performed efficiently by an Arnoldi procedure. The situation is different when general norms are considered, as the subspace optimization step involves non-convex and non-linear functions and thus requires a different strategy. Our major contributions are as follows: (a) we propose an iterative inner-optimization scheme that ensures a monotonic growth on the k-th Krylov-type subspace and involves matrices of smaller size than the original A, (b) we show ascent in

the objective function and convergence to a critical value for any matrix A and (c) we prove a global convergence theorem for a class of entry-wise nonnegative matrices A that generalizes to any pair of differentiable and absolute norms and extends to the new method the fundamental global convergence property of the original power method.

Francesco Tudisco
Dept. of Mathematics
University of Padua
tudisco.francesco@gmail.com

Antoine Gautier
Saarland University
ag@cs.uni-saarland.de

Matthias Hein
Saarland University
Dept. of Mathematics and Computer Science
hein@cs.uni-saarland.de

CP28

Fast and Backward Stable Computation of Roots of Polynomials

A stable algorithm to compute the roots of polynomials in the monomial basis is presented. Implicit QR steps are executed on a suitable representation of the iterates, which remain unitary plus low rank. The computational complexity is reduced to a minimum by exploiting the redundancy present in the representation allowing to ignore the low rank part. By ignoring the low rank part the remaining computations are solely based on rotations and thus unitary.

Thomas Mach
KU Leuven
Belgium
thomas.mach@nu.edu.kz

Jared Aurentz
Instituto de Ciencias Matemáticas
jaredaurentz@gmail.com

Raf Vandebril
Katholieke Universiteit Leuven
Department of Computer Science
raf.vandebril@cs.kuleuven.be

David S. Watkins
Washington State University
Department of Mathematics
watkins@math.wsu.edu

CP29

Terminal Regions and Costs for Discrete Time Quasi-Infinite Horizon NMPC

Terminal properties are essential to the stability of Nonlinear Model Predictive Control (NMPC). Here we develop a direct method to determine the terminal region and cost that guarantees asymptotic stability for NMPC of discrete time systems. Key to this analysis is the embedding of a fictitious linear discrete time controller that bounds the nonlinearities of the discrete time system within the determined terminal region. This approach extends previous work for continuous time NMPC [Chen and Allgower, A Quasi-Infinite Horizon Nonlinear Model Predictive Con-

trol Scheme with Guaranteed Stability, 1998][Rajhans et al, Two Alternative Approaches for Characterization of the Terminal Region for Continuous Time Quasi-Infinite Horizon NMPC, 2016], but it has more general applications, as it does not require small discrete step sizes to approximate the continuous dynamic system. In particular, larger steps selected for the application allows more computationally intensive NMPC models to be considered. In addition to determining the terminal region, we also show how a suitable horizon length is related to the discrete step size, terminal cost, and terminal region. The results of the stability analysis, along with computational performance of this approach will be demonstrated on a quadruple-tank process [Raff et al, Nonlinear Model Predictive Control of a Four Tank System: An Experimental Study, 2006], and will be compared with previous work for continuous systems.

Devin W. Griffith, Lorenz Biegler
Carnegie Mellon University
Department of Chemical Engineering
dwgriffi@andrew.cmu.edu, lb01@andrew.cmu.edu

CP29
Convexity in Hamilton-Jacobi Theory with Measurable Time-Dependence

Value functions propagated from initial or terminal costs and constraints by way of a differential inclusion, or more broadly through a Lagrangian that may goes to infinity, are studied in the case where convexity persists in the state argument. This paper examines the value function with associated Lagrangian being measurably time-dependent. For such value functions, we cannot take the subgradient by the point evaluation, instead by the essential values of the Hamiltonians. Furthermore, we demonstrate that such value functions satisfy a subgradient form of the Hamilton-Jacobi equations. Close relations with a dual value function are revealed.

Qingxia Li
Fisk University
qli@fisk.edu

CP29
Hub Network Design under Stackelberg Game for Time-Definite Delivery Industry

The industry provides services for shippers' time-sensitive small shipments. Under the duopolistic Stackelberg market, the leader may determine its hub network together with the market price to maximize its own profit under the notation that the follower is price takers. We used time-definite delivery industry in Taiwan as numerical example. The results for Nash and Stackelberg games will be discussed.

Cheng-Chang Lin
National Cheng Kung University
cclin@mail.ncku.edu.tw

CP29
A Novel Parallel Approach for Orthogonal Constrained Optimization Problems

To construct parallel approach for solving orthogonal constrained optimization problems is usually regarded as impossible mission, due to the low scalability of orthogonalization procedure. In this talk, we propose a Jacobi type column-wise block coordinate descent method for solving a class of orthogonal constrained optimization problems, and establish the global iterate convergence to stationary point of our proposed approach. A distributed algorithm is consequently implemented. Numerical experiments illustrate that the new algorithm has brilliant performance and high scalability in solving discretized Kohn-Sham total energy minimization problems.

Xin Liu
Academy of Mathematics and Systems Science
Chinese Academy of Sciences
liuxin@lsec.cc.ac.cn

MS1
Using Case Studies In A Diversity Training

This talk will briefly outline the use of case studies for diversity trainings in a mathematics department, for instructors (faculty and graduate students) and for undergraduate course assistants: what has worked, what hasn't worked so well, how to give one, attitudes of the trainees, etc. But most of the talk will actually consist of looking at such a case study. Attendees will be asked to discuss a fictional situation, inspired by true events, that reflects difficulties a student from an underrepresented group might face, and what support we as faculty, advisors or instructors can offer. Come with an open mind, a willingness to hear others' points of view and to share yours, and a respectful and constructive attitude. We hope this will prove a learning experience for us all, and that attendees can then lead such a training at their institution.

Rosalie Belanger-Rioux
Harvard University
Department of Mathematics
rbr@math.harvard.edu

MS1
Providing Opportunities for Low-Income Math Students With Academic Promise

The Scholarships in Science, Technology, Engineering, and Mathematics (S-STEM) program at the National Science Foundation (NSF) provides awards to institutions of higher education in totaling from $650,000 up to $5,000,000 (over 5 years) to develop programs that will support STEM degree attainment by low-income students who have demonstrated academic promise and financial need. At least 60% of the award funds must go directly to students, in increments not to exceed $10,000 per year per student. Some examples of successful S-STEM projects that focus on mathematics and tailored information about preparing a strong S-STEM proposal will be provided by an NSF program officer. S-STEM is part of NSFs portfolio of Broadening Participation programs.

Ron Buckmire
National Science Foundation
rbuckmir@nsf.gov

MS1
Accessibility for Mathematicians with Hearing Loss

More people with hearing loss are studying mathematics or using it in their teaching or research by taking advantage of amplification technologies such as hearing aids and cochlear implants and accessibility legislation. While not all remain in mathematics, some go on to hold leadership positions in STEMM (Science, Technology, Engineering,

Mathematics and Medicine). As these achievements indicate the potential for people with hearing loss to succeed in acquiring mathematical knowledge, it is opportune to describe how mathematics can be made more accessible at colleges and universities. People with hearing loss struggle with reduced access to auditory information and have to deal with societal challenges of isolation, ignorance, and invisibility. In USA, the proportion of people in STEMM with hearing loss is extremely small ($\sim 1\%$). Two challenges - invisibility and isolation - cause hearing loss to be underreported. So it helps to know about and network with mathematicians with hearing loss. Ignorance is due to lack of information about dealing with hearing loss, so it is important to self-advocate for accessibility. Accessibility should focus on three things: acoustic environment, technology and creating personalized solutions. Having more people with hearing loss in mathematics, aided by advances in amplification and pedagogy, has the potential for new ideas and concepts in mathematics to emerge to the benefit of everyone.

J T Ratnanather
Johns Hopkins University
tilak@cis.jhu.edu

MS1
Promoting Diversity in Mathematics: Bringing the Community into Conversations and Action

Horizons is a new seminar at Brown University organized by members of the math department dedicated to the following goals: to discuss issues of gender, racial, and sexual inclusivity in STEM fields; to provide career advancement advice to graduate students; and to promote the research and work of traditionally underrepresented mathematicians. Since its first event in 2016 fall, the seminar has enjoyed great attendance and sparked conversations among students and faculties across multiple departments on campus. In this talk, I will share the founding story of the Horizons seminar, where the idea originated, how it came to realization, and the success and challenges we have faced throughout the past year. In particular, I will highlight the transformation of the roles of our community during this process and the positive chain effect this seminar has created among the STEM departments at Brown.

Sunny Xiao
Brown University
yang_xiao@brown.edu

MS2
Numerical Posterior Distribution Error Control and Expected Bayes Factors

Abstract Not Available At Time Of Publication.

Marcos A. Capistran
CIMAT A.C.
Mexico
marcos@cimat.mx

J. Andrés Christen
CIMAT, Mexico
jac@cimat.mx

Miguel A. Moreles
Centro de Investigacion en
Matematicas
moreles@cimat.mx

MS2
Accelerating Markov Chain Monte Carlo with Active Subspaces

Abstract Not Available At Time Of Publication.

Paul Constantine, Carson Kent
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu, ckent@mines.edu

Tan Bui-Thanh
The University of Texas at Austin
tanbui@ices.utexas.edu

MS2
Derivative-Informed Mcmc for Bayesian Calibration of Stochastic Pde Models

Abstract Not Available At Time Of Publication.

Umberto Villa
University of Texas at Austin
uvilla@ices.utexas.edu

Omar Ghattas
The University of Texas at Austin
omar@ices.utexas.edu

MS2
Efficient Evaluation of Rare Event Probabilities Using Bayesian Inference

We consider the problem of estimating rare event probabilities, focussing on systems whose evolution is governed by differential equations with uncertain input parameters. If the system dynamics is expensive to compute, standard sampling algorithms such as the Monte Carlo method may require infeasible running times to evaluate these probabilities to a specified accuracy level. We propose a variance reduction scheme (called BIMC) that relies on solving a sequence of Bayesian inverse problems. The information gleaned from Bayesian inversion, namely, MAP points and the Hessians of the negative logarithm of the posterior distribution, is used to identify regions of the parameter space where the rare event occurs. Next, we construct local Gaussian approximations to the posterior PDFs at the MAP points. These Gaussians are then collected together to form an importance distribution. We apply BIMC to several real and synthetic systems and demonstrate that it can lead to computational savings of several orders of magnitude over the Monte Carlo method. Successful Bayesian inversion is a crucial component of our algorithm. We also present a case when our algorithms fail due to the poor quality of the inverse problem solution.

Siddhant Wahal
The university of Texas at Austin
siddhant@ices.utexas.edu

George Biros
The Institute for Computational Engineering and Sciences
The University of Texas at Austin

biros@ices.utexas.edu

MS3

A New Convergence Analysis of Finite Element Methods for Elliptic Distributed Optimal Control Problems with Pointwise State Constraints

We will discuss finite element methods for elliptic distributed optimal control problems with pointwise state constraints on two and three dimensional convex polyhedral domains formulated as fourth order variational inequalities.We will present a new convergence analysis that is applicable to C^1 finite element methods, classical nonconforming finite element methods and discontinuous Galerkin methods.

Susanne Brenner
Department of Mathematics
Louisiana State University
brenner@math.lsu.edu

MS3

Super-convergence of the Asymptotic Approximation of Linear Kinetic Equation with Spectral Methods

In this work, 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 domain in the system. 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 ℓth 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. Numerical tests will also be presented to support the theoretical results.

Zheng Chen
Oak Ridge National Laboratory
chenz1@ornl.gov

MS3

Numerical Methods for the Chemotaxis Models

In this talk, we will introduce and discuss several recently developed numerical methods for the approximation and simulation of the chemotaxis and related models in Biology. Numerical experiments to demonstrate the stability and high-order accuracy of the proposed methods for chemotaxis systems will be presented. Ongoing research projects will be discussed as well.

Yekaterina Epshteyn
Department of mathematics
University of Utah

epshteyn@math.utah.edu

MS3

The Effect of the Sensitivity Parameter in Weighted Essentially Non-oscillatory Methods

Weighted essentially non-oscillatory methods (WENO) were developed to capture shocks in the solution of hyperbolic conservation laws while maintaining stability and without smearing the shock profile. WENO methods accomplish this by assigning weights to a number of candidate stencils, according to the smoothness of the solution on the stencil. These weights favor smoother stencils when there is a significant smoothness difference, while combining all of the stencils to attain higher order when the stencils are all smooth. When WENO methods were initially developed, a small parameter ϵ was introduced to avoid division by zero. Over time, it has become apparent that ϵ plays the role of the sensitivity parameter in the stencil selection. In addition, the oscillations in the numerical solution also depend on the size of ϵ. In this talk I will show that the value of ϵ must be below a certain critical threshold ϵ_c, the dependence of this threshold on the function used and on the size of the jump discontinuity captured. I will also discuss some results about the size of the oscillations when $\epsilon < \epsilon_c$, and their dependence on the size of ϵ, the function used, and the size of the jump discontinuity. This work is joined with Bo Dong, Sigal Gottlieb, Yan Jiang, and Haijin Wang.

Yulia Hristova
University of Michigan-Dearborn
yuliagh@umich.edu

MS5

Learning Influence Structure Among Variables: An Interventional Measurement Approach

Abstract Not Available At Time Of Publication.

Negar Kiyavash
UIUC
kiyavash@illinois.edu

MS5

Rate-Optimal Estimation of High Dimensional Time Series

Abstract Not Available At Time Of Publication.

Han Liu
Princeton University
hanliu@princeton.edu

MS5

Nonlinear Autoregressive Point Processes

Poisson autoregressive models are a common way of capturing self-exciting point processes, where events from nodes in a network either stimulate or inhibit events from other nodes. These models can be used to learn the structure of social or biological neural networks. However, ensuring stability in these models can require overly restrictive assumptions on the network structure. We will consider a generalization of the PAR model which permits nonlinear dampening effects. Such a model allows for self-excitation while avoiding exponential blow-up in event counts, but

the introduction of nonlinearities brings new challenges in the analysis.

Benjamin Mark
UW-Madison
bmark2@wisc.edu

MS5

Lasso Guarantees for High Time Dimensional Time Series Estimation under Mixing Conditions

The Lasso is one of the most popular methods in high dimensional statistical learning. Most existing theoretical results for the Lasso, however, require the samples to be iid. Recent work has provided guarantees for the Lasso assuming that the time series is generated by a sparse Vector Auto-Regressive (VAR) model with Gaussian innovations. Proofs of these results rely critically on the fact that the true data generating mechanism (DGM) is a finite-order Gaussian VAR. This assumption is quite brittle: linear transformations, including selecting a subset of variables, can lead to the violation of this assumption. In order to break free from such assumptions, we derive non-asymptotic inequalities for estimation error and prediction error of the Lasso estimate of the best linear predictor without assuming any special parametric form of the DGM. Instead, we rely only on (strict) stationarity and mixing conditions to establish consistency of the Lasso in the following two scenarios: (a) α-mixing Gaussian processes, and (b) β-mixing sub-Gaussian random vectors. Our work provides an alternative proof of the consistency of the Lasso for sparse Gaussian VAR models. But the applicability of our results extends to non-Gaussian and non-linear times series models.

Ambuj Tewari
University of Michigan
tewaria@umich.edu

MS6

Analytic Lie Symmetric Solutions of Nonlinear Partial Differential Equations

A mixed Lie symmetry and direct method is presented for nonlinear differential equations. The nonlinear differential equations are invariant under translations in the independent variables. The Power Index method tests whether certain hyperbolic or Jacobian elliptic functions are analytic solutions. The basis for the G/G method is discussed and the nature of the expanded set of solutions analyzed. Both methods realize an aim of Sophus Lie to find analytic solutions of nonlinear differential equations.

Barbara Abraham-Shrauner
Department of Electrical and Systems Engineering
Washington University in St. Louis
bas@wustl.edu

MS6

Nonclassical Symmetries of a Nonlinear Diffusion-Convection/Wave Equation and Equivalents System

It is generally known that classical point and potential Lie symmetries of differential equations (the latter calculated as point symmetries of an equivalent system) can be different. We question whether this is true when the symmetries are extended to nonclassical symmetries. In this talk we consider two classes of nonlinear partial differential equations; the first one is a diffusion-convection equation, the second one a wave equation where we will show that the majority of the nonclassical point symmetries are included in the nonclassical potential symmetries. We highlight a special case were the opposite is true.

Danny Arrigo
Department of Mathematics
University of Central Arkansas
darrigo@uca.edu

MS6

Nonclassical Symmetry Solutions of Useful Nonlinear Reaction-Diffusion Equations in N Dimensions

For nonlinear reaction-diffusion equations in n spatial dimensions, there is a single restriction relating nonlinear diffusivity to nonlinear reaction, that always allows nonclassical symmetry reduction to a linear PDE. This allows us to construct (1) A class of unsteady solutions to a reaction-diffusion equation with Arrhenius reaction term for combustion, that follows from the Gibbs non-analytic temperature-dependent probability distribution. (2) A class of unsteady solutions to a reaction-diffusion equation with Fisher or Fitzhugh-Nagumo population growth terms, (3) A class of unsteady solutions for water flow in unsaturated soil, with logistic plant-root extraction terms.

Phil Broadbridge
School of Engineering and Mathematics Sciences
La Trobe University
p.broadbridge@latrobe.edu.au

MS6

Lie and Conditional Symmetries of Some Multicomponent Systems of Nonlinear Evolution Equations and Their Application for Constructing Exact Solutions

Lie and Q-conditional (nonclassical) symmetries of some multicomponent systems of PDEs (including diffusive Lotka–Volterra system) arising in population dynamics are under study. The Lie symmetry classification problems are completely solved. Moreover, a wide range of Q-conditional symmetries are solved. Notably, non-Lie symmetries (in an explicit form) for multi-component nonlinear reaction-diffusion systems are constructed for the first time. The symmetries obtained are applied for Lie and non-Lie reduction of two three-component systems, which are used for modeling interactions between three species in population dynamics. Exact solutions describing different scenarios of interaction between three species are constructed and their biological interpretation is discussed.

Roman Cherniha
Institute of Mathematics
National Acad.Sci. of Ukraine
r.m.cherniha@gmail.com

MS7

Asynchronous Iterative Solvers for Extreme-Scale Computing

Massive exascale parallelism will pose challenges to the efficient execution of numerical codes that use global synchronization or a bulk synchronous parallel model of computation. This is because any load imbalance or non-

uniformity in hardware performance will cause all processing units to idle at a synchronization point, waiting for the slowest unit. We focus on an asynchronous approach for the iterative methods used in existing large-scale codes. One idea is to replace outer Krylov subspace solvers with an asynchronous optimized Schwarz method. Subdomain solves in the optimized Schwarz method use a preconditioned Krylov subspace method. Thus the Krylov subspace method is moved to an inner level, acting on subdomains whose sizes are chosen such that performance non-uniformities are small or can be tolerated. This project is funded by the U.S. Department of Energy Office of Science, Office of Advanced Scientific Computing Research, Applied Mathematics program.

Edmond Chow
School of Computational Science and Engineering
Georgia Institute of Technology
echow@cc.gatech.edu

Erik G. Boman
Center for Computing Research
Sandia National Labs
egboman@sandia.gov

Jack J. Dongarra
University of Tennessee, Oak Ridge National Laboratory, USA
dongarra@icl.utk.edu

Daniel B. Szyld
Temple University
szyld@temple.edu

MS7
Communication Avoiding Iterative Methods and NLAFET Project

In this talk we discuss iterative methods and preconditioners that allow to reduce the communication cost of classic Krylov subspace methods and hence are more suitable for massively parallel computers. Our approach relies on enriching the subspace used in these methods that allows, at the cost of some extra computation, an important reduction in communication, while leading to a much faster convergence than classic Krylov methods. We also discuss the design of communication avoiding preconditioners to accelerate the convergence of iterative methods. This work is performed as part of the NLAFET project.

Laura Grigori
INRIA
France
Laura.Grigori@inria.fr

MS7
Inexact Coarse Solvers For Adaptive Preconditioners Using Block Recycled Iterative Methods

In this talk, I will present some recent algorithmic advances to improve the scalability of existing domain decomposition methods that use Galerkin coarse grid operators. The three main parts of the presentation will deal with: 1) multilevel overlapping Schwarz methods, 2) coarse grid preconditioners with mixed-precision arithmetic, and 3) domain decomposition methods with enlarged Krylov subspaces, i.e.,with multiple search directions.I'll show numerical results on a variety of examples (elliptic, saddle point, and frequency domain problems) and present some technical details of the implementation in the open-source framework HPDDM (https://github.com/hpddm/hpddm).

Pierre Jolivet
CNRS
pierre.jolivet@enseeiht.fr

MS7
Factorization Based Sparse Solvers and Preconditioners for Exascale

Factorization based algorithms are often the most robust algorithmic choices for solving linear systems from multiphysics and multiscale simulations, being used as direct solvers, or as coarse-grid solvers in multigrid, or as preconditioners for iterative solvers. We present our recent research on novel factorization algorithms incorporating data-sparse low-rank structures, such as hierarchical matrix algebra, to achieve lower arithmetic and communication complexity. We will illustrate both theoretical and practical aspects of the methods, and demonstrate their performance on new manycore machines.

Xiaoye S. Li, Pieter Ghysels
Lawrence Berkeley National Laboratory
xsli@lbl.gov, pghysels@lbl.gov

Christopher Gorman
Univ. of California, Santa Barbara
gorman@math.ucsb.edu

Francois-Henry Rouet
Livermore Software Technology Corp.
fhrouet@lstc.com

MS8
Krylov Subspace Spectral Methods for Navier-Stokes in Cylindrical Geometries

Existing time-stepping methods for PDEs such as Navier-Stokes equations are not as efficient or scalable as they need to be for high-resolution simulation due to stiffness. The failure of existing time-stepping methods to adapt to changes in technology presents a dilemma that is becoming even more problematic over time. By rethinking approaches to time-stepping, dramatic gains in efficiency of simulation methods can be achieved. Krylov subspace spectral (KSS) methods have proven to be effective for solving time-dependent, variable-coefficient PDEs. The objective of this research is to continue the development of KSS methods to provide numerical solution methods that are far more efficient and scalable to high resolution for Navier-Stokes equations. So far, KSS methods have been applied only on 1-dimensional, 2-dimensional, and 3-dimensional rectangular domains, but current work is extending them to polar domains using polar coordinates and expansions in Legendre polynomials instead of Fourier series. We will utilize these techniques for Navier-Stokes equations on rectangular domains as well as polar domains.

Brianna Bingham
The University of Southern Mississippi
brianna.bingham@usm.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics

James.Lambers@usm.edu

MS8

Scalable Computation of Matrix Functions for Time-Dependent Pdes Through Asymptotic Analysis of Block Krylov Projection

Exponential propagation iterative (EPI) methods provide an efficient approach to solving large stiff systems of ODE, compared to standard integrators. However, the bulk of the computational effort in these methods is due to products of matrix functions and vectors, which can become very costly at high resolution due to an increase in the number of Krylov projection steps needed to maintain accuracy. In this presentation, EPI methods are modified by using Krylov subspace spectral (KSS) methods, instead of standard Krylov projection methods, to compute products of matrix functions and vectors. Numerical experiments show that this modification causes the number of Krylov projection steps to become bounded independently of the grid size, thus dramatically improving efficiency and scalability.

Alex Cibotarica
Ivy Tech Community College
cialex@yandex.ru

MS8

A Smoothed Radial Point Interpolation Implicit Method for Heat Conduction Based on the Element-by-Element Technique

The smoothed radial point interpolation methods (S-RPIM) have been well-used for solving heat conduction problems. The weakened weak (W2) formulation ensures that radial point interpolation method can be used to create the shape functions, which makes the S-RPIM more accuracy and robust than the finite element method (FEM) based on the same triangular/tetrahedral background meshes. However, since more points are used for interpolation, the conductivity matrix of S-RPIM is denser than that of FEM. Therefore, the cost for equation solving would be expensive when implicit schemes are used. In this presentation, we apply the idea of the element-by-element to S-RPIM for solving 2D heat transfer problems. Even though the Crank-Nicolson scheme is used, the problems can be solved by smoothing domain without assembling the global conductivity matrix. The computational accuracy and efficiency of the proposed method are tested by comparing it with the original S-RPIM.

Wen Li, Guagming Yao
Clarkson University
liw2@clarkson.edu, gyao@clarkson.edu

MS8

Local Radial Basis Function Method for Quenching Problem

For time-dependent problems that the solutions become infinite in finite time irrespective of initial values, there usually exists a parameter, so called critical value, that makes the problem blow-up in finite time. As the critical values generally cannot be computed analytically, especially when the domain of the PDE is complicated, we usually resort to numerical methods to approximate. In the past, both the finite element method (FEM) and boundary element method (BEM) have been used for this purpose. Some papers reported results for quenching problems using meshless method, such as method of fundamental solutions (MFS). In this presentation, we will use a local radial basis function method, so called the method of particular solutions (MPS) to find the critical values of some quenching problems.

Guagming Yao, Wen Li
Clarkson University
gyao@clarkson.edu, liw2@clarkson.edu

MS9

Modeling the Spread of Ebola with SEIR and Optimal Control

We use an SEIR model to simulate the transmission of the 2014 Ebola virus. Optimal control theory is used to explore the effects of vaccination and quarantine rates on the model.

Harout Boujakjian
George Mason University
haroutb719@gmail.com

MS9

Equivalence of n-th Order Difference Equations Under Point Transformations

Given two n-th order finite difference equations, we will determine if there exists an invertible map sending one equation onto the other using the new method of equivariant moving frames.

Jonathan D. Colon
SUNY New Paltz
Colonj1@hawkmail.newpaltz.edu

MS9

Numerical Phase Retrieval From Power Spectra of Deterministically Masked Signals

Research is ongoing on developing algorithms for reconstructing a signal from its power spectrum, a problem that arises particularly in diffraction imaging. In general, this inverse problem is difficult to solve without prior knowledge of the signal. One of the methods recently developed for reconstruction of any input has been using masks during measurement to distort the signal in different ways, to create redundancy, and, using a polarization method, to determine the original signal up to difference in global phase. This method employs knowledge of spectral graph theory with Fourier analysis to construct random masks that will enable polarization recovery of any signal with high probability. We will explore a numerical implementation of this algorithm, its stability and efficiency, and the possibility of improvements using an additive combinatorics result to deterministically create masks for polarization recovery.

Nicholas Frederick, Sami Merhi
Michigan State University
frede123@msu.edu, merhisam@math.msu.edu

MS9

A Multicompartment Mathematical Model of Neuroblastoma Tumor Growth

We designed a simple mathematical model for neuroblastoma growth that uses a system of ordinary differ-

ential equations to model qualitative results observed in xenograft in vivo culture.

Yixuan He
Dartmouth College
yixuan.he.18@dartmouth.edu

MS9
Trend to Equilibrium for a Delay Vlasov-Fokker-Planck Equation and Explicit Decay Estimates

Motivated by models describing the lay-down of fibers in textile production processes we consider a delay Vlasov-Fokker-Planck equation and the associated stochastic interacting particle system with delay and investigate them analytically. Under certain restrictions on the parameters well-posedness and ergodicity of the mean-field equation are shown and an exponential rate of convergence towards the unique stationary solution is proven as long as the delay is finite. For infinte delay i.e., when all the history of the solution paths are taken into consideration polynomial decay of the solution is shown.

Lisa M. Kreusser
University of Kaiserslautern
lmk48@cam.ac.uk

MS9
Modeling-Backed Microwave Imaging in Closed Systems: Reconstruction of a Spherical Inhomogeneity

Microwave imaging is currently under extensive development as a potential alternative to the traditional NDE/NDT techniques that may perform safer, more accurate, and more cost-effective evaluations. This work continues a series of studies demonstrating feasibility of using modeling data in microwave imaging conducted in closed microwave systems. We propose a computational procedure in support of elementary measurement of reflection and transmission coefficients that finds spatial coordinates (In earlier technique), and introduces the determination of radius and dielectric constant and the loss factor of a spherical object hidden inside a dielectric sample located in a cavity with multiple waveguide inputs. Reconstruction is based on a neural network inversion and backed by data from 3-D FDTD analysis. In order to improve accuracy of the model, special measures are taken in FDTD discretization, and the network is expanded by adding the inputs corresponding to reflection and transmission at two additional frequencies. Functionality of the proposed technique is illustrated by computational tests in finding characteristics of a spherical inclusion in a rectangular Teflon block located in a Magic Tees waveguide junction. The output of this work has initiated an implementation of the technique in a physical prototype; the experimental program is sponsored by MACOM, measurements are being conducted in the McMaster University.

Taylor J. York
Worcester Polytechnic Institute
tjyork@wpi.edu

MS10
Bayesian Inference for an Estimating Discrepancy Functions in Turbulence Models

Due to their computational efficiency, Reynold-Averaged Navier-Stokes (RANS) turbulence models remain a vital tool for modeling turbulent flows. However, it is well known that RANS predictions are locally corrupted by epistemic model-form uncertainty. We therefore wish to perturb the Reynold-stress tensor at locations in the flow domain where the modeling assumptions are likely to be invalid. However, inferring such perturbations at every location in the computational mesh leads to a high-dimensional inverse problem. To make the problem scalable, we propose two additional transport equations for the Reynolds-stress perturbations, such that their spatial structure is now pde-constrained. Exploring the posterior distribution of the Reynolds-stresses can now be achieved through a low-dimensional Bayesian inference procedure on the coefficients of the perturbation model. We will demonstrate our framework on a number of canonical flow problems where RANS models are prone to failure.

Wouter N. Edeling
TU Delft
wedeling@stanford.edu

Gianluca Iaccarino
Stanford University
Mechanical Engineering
jops@stanford.edu

MS10
Bayesian Uncertainty Quantification in Numerical Integration

Abstract Not Available At Time Of Publication.

Briol Francois-Xavier
The University of Warwick
f-x.briol@warwick.ac.uk

MS10
QMC with Product Weights for Elliptic PDEs with Coefficients Parametrized in Multiresolution Representations

Parametric diffusions are considered with coefficients that are given by multiresolution representations. Approximations by QMC with randomly shifted lattice rules for first order and with interlaced polynomial lattice rules for higher order are analyzed with dimension independent convergence rates. The so called affine and lognormal case for the parametric coefficient are discussed. The local support structure in the multiresolution expansion are known to imply product weights for QMC rules, cp. [Gantner, Herrmann, Schwab, SAM-report 2016-32, ETH Zuerich] and [Herrmann, Schwab, SAM report 2016-39, ETH Zuerich]. Product weights allow for linear scaling in the dimension of integration in the cost to create QMC rules by the CBC construction, cp. [Nuyens, Cools, Math. Comp., 75(254):903920, 2006]. Multilevel QMC quadratures are considered to reduce the work of the QMC approximation in general polyhedral spatial domains, cp. [Gantner, Herrmann, Schwab, SAM-report 2016-54, ETH Zuerich] and [Herrmann, Schwab, SAM report 2017-04, ETH Zuerich].

Lukas Herrmann, Robert N. Gantner
ETH Zurich
lukas.herrmann@sam.math.ethz.ch,
robert.gantner@sam.math.ethz.ch

Christoph Schwab
ETH Zuerich
SAM

christoph.schwab@sam.math.ethz.ch

MS10
Optimal Parameter Dimension Reduction for Nonlinear Bayesian Inverse Problems

Abstract Not Available At Time Of Publication.

Olivier Zahm
Massachusetts Institute of Technology
zahmo@mit.edu

MS11
A Moving Mesh WENO Method Based on Exponential Polynomials for One-dimensional Conservation Laws

We develop a novel WENO scheme with non-polynomial bases, in particular, the exponential bases, with a high order moving mesh method for one-dimensional (1D) hyperbolic conservation laws, which is shown to be effective in resolving shocks and other complex solution structures. A collection of numerical examples is presented to demonstrate high order accuracy and robustness of the method in capturing smooth and non-smooth solutions, including the strong δ shock arising from the weakly hyperbolic pressureless Euler equations.

Yan Jiang
Michigan State University
jiangyan@math.msu.edu

MS11
Pseudo-time Adaptive Regularization for Nonmonotone Problems

We will discuss some of the unique challenges encountered in approximating the solutions to elliptic partial differential equations of nonmonotone type. Starting simulations on a coarse mesh, for the ultimate efficiency of the method, may trigger a sequence of divergent iterates based on linearized problems, unless some type of stabilization, or regularization is introduced. We will discuss adaptive strategies based on pseudo-time regularization to produce convergent sequences of iterates to approximate the PDE solution. The talk will be illustrated with numerical examples of the developed ideas applied to finite element discretizations of nonlinear diffusion problems.

Sara Pollock
Wright State University
sara.pollock@wright.edu

MS11
On the Sensitivity to the Filtering Radius in Leray Models of Incompressible Flow

One critical aspect of Leray models for the Large Eddy Simulation (LES) of incompressible flows at moderately large Reynolds number (in the range of few thousands) is the selection of the filter radius. This drives the effective regularization of the filtering procedure, and its selection is a trade-off between stability (the larger, the better) and accuracy (the smaller, the better). In this paper, we consider the classical Leray-alpha and a recently introduced Leray model with a deconvolution-based indicator function, called Leray-alpha-NL. We investigate the sensitivity of the solutions to the filter radius by introducing the

sensitivity systems, analyzing them at the continuous and discrete levels, and numerically testing them on two benchmark problems.

Annalisa Quaini
Department of Mathematics, University of Houston
quaini@math.uh.edu

MS11
A BDDC Preconditioner for C^0 Interior Penalty Methods

A balancing domain decomposition by constraints (BDDC) algorithm is constructed and analyzed for a discontinuous Galerkin method, the C^0 interior penalty method, for biharmonic problems. The condition number of the preconditioned system is bounded by $C(1+\ln(H/h))^2$, where h is the mesh size of the triangulation, H is the typical diameter of subdomains, and the positive constant C is independent of h and H. Numerical experiments corroborate this result.

Kening Wang
University of North Florida
kening.wang@unf.edu

MS13
Motion Control and Coordination of Underactuated Bodies in An Ideal Fluid

Hydrodynamic coupling between discrete underactuated bodies in an ideal fluid produces simple interactions between the bodies, such as attraction, repulsion, and synchronization. In this work we exploit this intra-body coupling to actively command desired trajectories in the workspace. Such trajectories may be the result of stitching together the aforementioned motion primitives, and they may also involve the coordination of simultaneous actuation in more than one body. We also consider problems in which certain bodies remain passive with no internal actuation, such that their locomotion is purely due to interactions with other bodies. In previous work we developed a simple model that approximates the resultant flow between two bodies as a linear combination of movement components in two orthogonal directions. We extend this technique to a system with more than two bodies in order to analytically pose and solve a feasible motion planning problem.

Tony Dear
Robotics Institute
Carnegie Mellon University
tonydear@cmu.edu

MS13
Optimizing the Performance of Hydrofoils Coupled Through a Vortical Ideal Fluid

In previous work the authors demonstrated that for a pitching and heaving hydrofoil the use of a non-sinusoidal flapping gait can increase thrust or propulsive efficiency above that achieved by a purely sinusoidal gait. This work goes beyond a single immersed body to consider the self-propulsion of multiple hydrofoils coupled through an ideal fluid. Each hydrofoil sheds vorticity aft of its trailing edge so as to satisfy an appropriate Kutta condition and to conserve the system's net circulation. In addition to non-sinusoidal gaits, the effect on propulsive efficacy of relative actuation phases and spatial hydrofoil separations are discerned by varying the kinematic inputs and geometric con-

figurations of the hydrofoils. Numerical results obtained via a fast boundary-element panel method are presented, along with experimental results from a robotic array of coupled hydorfoils. This work was supported by the Office of Naval Research through MURI grant N00014-14-1-0533.

Michael J. Fairchild
Princeton University
mjf5@princeton.edu

Clarence Rowley
Princeton University
Department of Mechanical and Aerospace Engineering
cwrowley@princeton.edu

Rakshit Bhansali
University of North Carolina at Charlotte
rbhansal@uncc.edu

Scott D. Kelly
Mechanical Engineering and Engineering Science
University of North Carolina at Charlotte
scott@kellyfish.net

MS13

Synch Or Swim: Coordinating Robot Teams in Geophysical Flows

Lagrangian coherent structures (LCS) are important for quantifying transport phenomena and enable the prediction of various physical, chemical, and biological processes in the ocean. Since marine autonomous vehicles must operate with limited energy budgets, it makes sense for them to leverage the surrounding flow to minimize their energy expenditures. We show how LCS can be leveraged and exploited for planning time and energy optimal paths for autonomous vehicles and for rendezvous with other vehicles. We conclude with a discussion on how these structures can be tracked in real time by a robot team using only local flow measurements.

M. Ani Hsieh
Drexel University
m.hsieh@seas.upenn.edu

Shibabrat Naik
Engineering Science and Mechanics
Virginia Tech
shiba@vt.edu

Eric Forgoston
Montclair State University
Department of Mathematical Sciences
eric.forgoston@montclair.edu

Herbert Tanner
Department of Mechanical Engineering
University of Delaware
btanner@udel.edu

Philip Yecko
Montclair State University
philip.yecko@montclair.edu

MS13

Dynamics and Interactions of Wheeled Robots on

Movable Platforms

A substantial literature addresses the nonlinear dynamics of robotic devices that move over flat surfaces under the influence of nonintegrable velocity constraints. More than one canonical problem in planar mobile robotics concerns a device that can vary aspects of its internal geometry in order to effect locomotion relative to a stationary supporting platform. Complementary to this is the problem of a device with unactuated internal degrees of freedom that can be excited by the dynamic behavior of a supporting platform to induce locomotion. When directly actuated devices and unactuated devices share a common platform with inertial dynamics of its own, the coupling between devices can engender interactions reminiscent of those observed within systems of aquatic robots coupled through high-dimensional hydrodynamics. This talk will illustrate these ideas with a selection of simple examples involving wheeled robots with flexible joints or internal rotors.

Scott D. Kelly
Mechanical Engineering and Engineering Science
University of North Carolina at Charlotte
scott@kellyfish.net

MS14

Network Modeling of High-Dimensional Time Series in the Presence of Factors

Estimating network connectivity among multiple time series is an important problem in many economic and financial applications. Examples include macroeconomic forecasting, system-wide risk monitoring and portfolio optimization. Sparsity-inducing regularizers commonly used in high-dimensional statistics do not account for the presence of pervasive factors influencing the underlying dynamics. In this work, we address the problem of estimating the networks of intertemporal and contemporaneous connectivity among multiple time series in the presence of common factor processes. For models with observable factor processes, we propose a regularized maximum likelihood procedure to simultaneously estimate the factor loadings and the conditional independence structure among the idiosyncratic components. We investigate the theoretical properties of the proposed method under high-dimensional scaling, assess its performance via extensive numerical studies and demonstrate its advantage on a motivating example from financial econometrics. In the presence of latent factors, we propose a low-rank and sparse modeling strategy to estimate the network after accounting for the underlying common factors.

Sumanta Basu
University of Michigan
sumbose@cornell.edu

George Michailidis
Informatics Institute
University of Florida
gmichail@umich.edu

MS14

Vector Autoregressive Model Inference with Missing Data

High-dimensional time series data exist in numerous areas such as in finance, genomics, healthcare and neuroscience. An unavoidable aspect of all such datasets is missing data and dealing with this issue has been an important focus in

statistics. In this work, we consider a high-dimensional inference problem where a dynamical system, governed by a Gaussian vector autoregressive model, is only partially observed. The inference amounts to estimating a transition matrix which is assumed to be sparse. In such a scenario, where covariates are highly interdependent and partially missing, new theoretical challenges arise. While transition matrix estimation in vector autoregressive models has been studied in the literature, the missing data scenario requires separate efforts. Moreover, while the transition matrix estimation can be studied from a high-dimensional sparse linear regression perspective, the covariates are highly dependent and existing results on regularized estimation with missing data from i.i.d. covariates are not applicable. In fact, the interactions among covariates depend on the unknown transition matrix which makes the problem even harder. In this talk, we draw upon existing ideas in the literature and propose an approach for regularized estimation of the transition matrix for a large family of stable Gaussian processes using only partial observations. We further provide recovery guarantees and error bounds to illustrate the effectiveness of this approach.

Amin Jalali
UW-Madison
amin.jalali@wisc.edu

Rebecca Willett
University of Wisconsin-Madison
willett@discovery.wisc.edu

MS14

Differential Parameter Estimation, with Application to Changes

We consider the problem of estimating the difference in parameters of a pair of graphical model distributions. This has a wide set of applications, including estimating a nonstationary but piecewise constant graphical model distribution, and estimating generative model binary classifiers, among others. While a natural approach is to estimate the two graphical model distributions individually, this is highly sub-optimal in high-dimensional settings, particularly when the individual parameters themselves do not have any low-dimensional structure, whereas the difference in parameters do. While this has attracted a line of recent work, we show that a very simple estimator nonetheless has state of the art performance. Our analysis introduces a new notion of separability of loss functions, together with a novel analysis of convergence rates of estimators in ell_infty norm. We corroborate our results via applications to neuroscience and weather extremes.

Pradeep Ravikumar
Department of Computer Sciences
University of Texas, Austin
pradeepr@cs.utexas.edu

MS14

Network Reconstruction From High-Dimensional Ordinary Differential Equations (ODEs)

We consider the task of learning a dynamical system from high-dimensional time-course data. For instance, we might wish to estimate a gene regulatory network from gene expression data measured at discrete time points. We model the dynamical system non-parametrically as a system of additive ordinary differential equations. Most existing methods for parameter estimation in ordinary differential equations estimate the derivatives from noisy observations. This has been shown to be challenging and inefficient. We propose a novel approach that does not involve derivative estimation. We show that the proposed method can consistently recover the true network structure even in high dimensions, and we demonstrate empirical improvement over competing approaches.

Ali Shojaie
University of Michigan
ashojaie@uw.edu

MS15

Generalized Equivalence Transformations ForDifferential Equations Involving Specific Arbitrary Functions

A method for determining generalized equivalence transformations for differential equation systems involving arbitrary functions is presented. It applies to differential equation systems whose arbitrary functions involve all equations independent variables only. The method has been implemented as the maple routine GENDEGET and is based on the maple package DESOLV (by Carminati and Vu). Since this technique can be further adapted to find the equivalence transformations for the studied system, practically any symbolic manipulation program designed to find classical Lie symmetries can also be used to determine generalized equivalence transformations and equivalence transformations, respectively, without any modification of the program.

Nicoleta V. Bila
Fayetteville State University
nbila@uncfsu.edu

MS15

You Have a Mathematical Model: What's Next?

Your mathematical model is a system of either ordinary or partial differential equations. You may take a numerical approach to it, although arbitrary parameters are on your way, and you have to guess which numbers to replace them with. Indeed, a crunching number approach. Or you may look at the asymptotic behavior of solutions. However, to infinity and beyond may dismiss what happens in finite time. Therefore, the next wise thing to do is search for the symmetries of your system. They may be trivial, they may be hidden. However, it is symmetries that allows both a qualitative and even better quantitative analysis of your model, before going to infinity. Constructing Lagrangians and determining first integrals [M.C. Nucci, G. Sanchini, Symmetries, Lagrangians and Conservation Laws of an Easter Island Population Model, Symmetry 7 (2015) 1613], finding hidden linearity [M.C. Nucci, S. Post, Lie symmetries and superintegrability, J. Phys. A: Math. Gen. 45 (2012) 482001], and even deriving analytical solutions [M.S. Hashemi, M.C. Nucci, Nonclassical symmetries for a class of reaction-diffusion equations: the method of heir-equations, J. Nonlinear Math. Phys. 20 (2013) 44] are the natural consequences of symmetries, although not the only ones [M.C. Nucci, Ubiquitous symmetries, Theor. Math. Phys. 188 (2016) 1361]. We will show several examples, where symmetries are at work in different scientific fields.

Maria Clara Nucci
Dipartimento di Matematica e Informatica
Universita' di Perugia

mariaclara.nucci@unipg.it

MS15

Lie Point Symmetry Preserving Discretization of the Liouville Equation

This talk is part of a general program the aim of which is to approximate differential equations by difference systems that are invariant under the same Lie point symmetry group. Both the hyperbolic and the elliptic Liouville equations with their infinite dimensional symmetries are considered. This is joint work with D.Levi and L.Martina.

Pavel Winternitz
Centre de Recherches Mathématiques
Université de Montréal
wintern@crm.umontreal.ca

MS16

It's not an ExaHyPE, yet: ADER-DG on Tree-structured Meshes for an Exascale Hyperbolic PDE Engine

ExaHyPE is a project funded via the European Horizon 2020 initiative "towards exascale high performance computing". Our project's mision is to develop an exascale-ready engine to solve grand challenge problems that may be modelled via hyperbolic systems of PDEs. The resulting engine will strictly rely on high-order ADER-DG discretisation on dynamically adaptive, tree-structured Cartesian meshes. The presentation will give an overview of the project and its approach, and will show first results from the tackled applications in seismology and astrophysics.

Michael Bader
Technical University of Munich
bader@in.tum.de

MS16

Experiences with AMR Co-design from the Perspective of an Application using AMR

Co-design Centers established under the ECP project can act as intermediaries between software technologies and scientific applications desirous of using them. Adaptive mesh refinement (AMR) is a way to compress computational and memory footprint of an application without compromising the fidelity of results. AMR is used extensively in multiple domains. AMR co-design center aims to provide an interface for these applications that abstract away most of these applications' interactions with lower level software and hardware technologies. We present early experience of one ECP AMR based application, core-collapse supernovae, with AMR co-design efforts.

Anshu Dubey
Argonne National Laboratory
adubey@anl.gov

MS16

Hierarchical Computations on Manycore Architectures: The HiCMA Library

At extreme scale, fast multipole and closely related H-matrix methods may dominate in solving many linear systems arising from differential and integral equations, statistics, and machine learning possessing a combination of low arithmetic complexity, high arithmetic intensity, low communication complexity, and potential for relaxed synchrony. They are, however, complex to implement efficiently on SIMT-like hardware, which is the goal of the HiCMA project at KAUST. We report on work leading to such HBLAS for accelerators.

Kadir Akbudak
Bilkent University
kadir.cs@gmail.com

Ali Charara, David E. Keyes
KAUST
ali.charara@kaust.edu.sa, david.keyes@kaust.edu.sa

Hatem Ltaief, Aleksandr Mikhalev
King Abdullah University of Science & Technology (KAUST)
hatem.Ltaief@kaust.edu.sa,
aleksandr.mikhalev@kaust.edu.sa

George M Turkiyyah
King Abdullah University of Science and Technology
American University of Beirut
gt02@aub.edu.lb

MS16

Towards Exascale in High-Order Computational Fluid Dynamics

The complex nature of turbulent fluid flows implies that the computational resources needed to accurately model problems of industrial and academic relevance is virtually unbounded. Computational Fluid Dynamics (CFD) is therefore a natural driver for exascale computing and has the potential for substantial societal impact, like reduced energy consumption, alternative sources of energy, improved health care, & improved climate models. Extreme-scale CFD poses several cross disciplinary challenges e.g. algorithmic issues in scalable solver design, handling of extreme sized data with compression and in-situ analysis, resilience and energy awareness in both hardware and algorithm design. The wide range of topics makes exascale CFD relevant to a wider HPC audience, extending outside the traditional fluid dynamics community. This talk will summarise the work within the EU funded Horizon 2020 project ExaFLOW, which brings together leading CFD experts and users from both industry and academica: Partners include KTH Royal Institute of Technology (Sweden), Imperial College (UK), University of Southampton (UK), University of Edinburgh (UK), University of Stuttgart (Germany), and industrial partners McLaren (UK) & ACSC (Germany). The presentation will show sample results addressing key algorithmic challenges in CFD in order to facilitate simulations at exascale, e.g. accurate and scalable solvers, data reduction methods & strategies to ensure fault tolerance and resilience.

Philipp Schlatter
KTH Stockholm
pschlatt@mech.kth.se

MS17

Wavelet Regularized Solution of Laplace Equation in an Arbitrary Shaped Domain

A numerical method for the solution of interior Dirichlet problem for the two-dimensional Laplace equation in an arbitrary shaped bounded domain is presented. This domain

is embedded in a circular domain and, exploiting the idea of analytic continuation, an inverse problem is formulated and solved for the boundary values of the unknown function on the circular domain. The ill-conditioning, usually associated with such inverse problems, is easily handled by a wavelet regularization. Numerical results are presented for an ellipse and a hexagon.

Vani Cheruvu
Department of Mathematics and Statistics
The University of Toledo, Toledo, OH 43606
vani.cheruvu@utoledo.edu

MS17

Discrete Convolution Methods for Solving Differential Equations

Abstract Not Available At Time Of Publication.

Joseph Kolibal
University of New Haven
jkolibal@newhaven.edu

MS17

A New Adaptive Method Modified Knot Insertion for RBF Approximation

Knot insertion is a classic technique employed to enhance the accuracy of approximation in interpolation problems by adaptively increasing the number of data points. The idea of the new adaptive method, Modified Knot Insertion (MKI), is proposed in order to improve the boundary error behavior of RBF interpolations. As opposed to the original Franke knot insertion method, rather than using a small fixed value of shape parameter, the MKI method associated with Residue-Error Cross Validation (RECV) during each iteration to achieve accuracy up to two orders of magnitude higher than that achieved using pseudo random collocation points such as Halton points.

L.H. Kuo
University of West Florida, USA
lkuo@uwf.edu

MS17

Rapid Modification of Orthogonal Polynomials for Pdes in Polar and Cylindrical Geometries

The goal of this project is that if we are given a Jacobi matrix for some measure $d\lambda(x)$, we want to obtain the Jacobi matrix for a modification of that measure $d\tilde{\lambda}(x) = r(x)d\lambda(x)$, where $r(x)$ is a rational function. Then, by partial fractions, this means considering the case of $r(x)$ being the reciprocal of a linear or irreducible quadratic factor, or a repitition thereof. The existing methods for this type of modification are computationally expensive. Therefore, our goal is to develop a faster method based on inversion of the procedure for modifying measures by multiplying by such factors. The challenge in this project is that this inversion requires working around missing information, which can be accomplished by treating the missing information as parameters and making guesses that can be corrected through an iteration such as using a root-finding method.

Amber C. Sumner
University of Southern Mississippi
amber.sumner@usm.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS18

TBA Castillo-Chavez

Abstract Not Available At Time Of Publication.

Carlos Castillo-Chavez
Simon A Levin Mathematical, Computational and
Modeling Scien
Arizona State University
ccchavez@asu.edu

MS18

TBA Radunskaya

Abstract Not Available At Time Of Publication.

Ami Radunskaya
Pomona College
Mathematics Department
aer04747@pomona.edu

MS18

TBA Tapia

Abstract Not Available At Time Of Publication.

Richard A. Tapia
Rice University
Dept of Comp & Applied Math
rat@rice.edu

MS18

TBA Villalobos

Abstract Not Available At Time Of Publication.

Cristina Villalobos
School of Mathematical and Statistical Sciences
The University of Texas Rio Grande Valley
cristina.villalobos@utrgv.edu

MS19

Recovery Time of Backed up Traffic

This presentation will give an analytic approximation to the time required to clear up a congested road. Partial differential equations were used to model the traffic patterns. The first part of the research is devoted to developing the buildup in the context of a single traffic light on a one way road. The traffic lightens up allowing for the buildup to pass. This system is approximated to find an upper bound to the time that is required to allow the traffic to pass through.

Ryan L. Reading
The Ohio State University
reading.15@osu.edu

MS19

Optimization of Power Output in a Magnetohydro-

dynamic Generator

Abstract Not Available At Time Of Publication.

Michael T. Redle
Oregon State University
redlem@oregonstate.edu

MS19

Efficiency of Water Distribution in Water Poor Areas of the World

Markov chains are used to model many different dynamical systems such as the movement of traffic, the spreading of disease, and the volatility of financial assets. In this presentation, we construct a Markov model of the distribution of water in water poor areas of the world. Using current data about the water availability to individuals in these areas, we present the efficiency of the distribution process as well as examine various changes to that process and their effects on the efficiency. Then, we present what specific changes to these water distribution systems would be the most significant for the populations that they serve.

Mitchell E. Sailsbery
Brigham Young University
mitchell.sailsbery@gmail.com

MS19

A Study of Parallel Simulation Procedures for the Taylor-Green Vortex Problem Using PETSc

In computational fluid dynamics (CFD), problems often result in stiff matrices which are suited to iterative linear solvers. High-fidelity simulations with finely partitioned grids require the use of cluster machines and parallel processing, which introduces a host of implementation challenges. In this talk, we discuss a parallel, iterative CFD code implemented using the Portable, Extensible Toolkit for Scientific Computation (PETSc) with Krylov Subspace (KSP) methods and preconditioners (PC). In particular, we present simulation results of the Taylor-Green problem for counter-rotating vortex pairs using both PETSc KSP solvers and an already developed iterative CFD code. The use of PETScs distributed arrays and data communication is discussed. Grid size, Mach number, and Reynolds number are varied to investigate the effects on simulation results. The speed up and efficiency of the code are analyzed.

Nicholas W. Stegmeier
South Dakota State University
nicholas.stegmeier@jacks.sdstate.edu

MS19

The Behavior of the Phase Response Curve Near Bifurcations in a Neuronal Model

Many neuronal models appear to operate near both a Takens-Bogdanov and cusp bifurcation. From the normal form of this bifurcation, we developed a two-dimensional neural model that resembles the Fitzhugh-Nagumo model. Depending on parameters, the onset to repetitive firing can occur at a Hopf, saddle-node infinite cycle, or various homoclinic bifurcations. We explored the shape of the phase resetting curves near these bifurcations and the implications for features such as synchronization.

Vighnesh Viswanathan, Michael Block

University of Pittsburgh
viv12@pitt.edu, mib74@pitt.edu

MS19

Modeling Over-the-Counter Derivative Trading with and without Central Clearing Parties

Over-the-counter (OTC) derivatives are believed to have played a significant role in the 2008 financial crisis. In response to this, new regulations were written in 2010 that required OTC derivatives to be traded through Central Clearing Parties (CCPs). Theoretically, these regulations should induce a greater amount of stability in the system, though in reality the truth of this statement is unclear. This model seeks to elucidate the issue by utilizing probabilistic methods including Gibbs Sampling to sample different possible OTC derivative trading networks based on the small amount of data available to a regulator. These networks can then be tested with systemic risk analysis to better understand the stability of each type of network: a bilateral trading network without a CCP, a network with one CCP, and one with multiple CCPs. Then using the netting efficiency defined by Duffie and Zhu (2009), we analyze the three different kinds of networks and the assumptions used to sample these networks, to better understand if CCPs accomplish the goal of creating more stability in the OTC derivative trading network.

Natalie S. Wellen
Worcester Polytechnic Institute
nswellen@wpi.edu

MS20

Interactions of Elastic Cilia Driven by a Geometric Switch

Cilia, flexible hairlike appendages located on the surface of a cell, play an important role in many biological processes including the transport of mucus in the lungs and the locomotion of ciliated microswimmers. Cilia self-organize forming a metachronal wave that propels the surrounding fluid. To study this coordinated movement, we model each cilium as an elastic, actuated body whose beat pattern is driven by a geometric switch where the beat angle switches between two traps, driving the motion of the power and recovery strokes. The cilia are coupled to a viscous fluid using a numerical method based upon a centerline distribution of regularized Stokeslets. We first characterize the beat cycle and flow produced by a single cilium and then investigate the synchronization states between two cilia. Cilia that are initialized in phase eventually lock into antiphase motion unless a additional velocity dependent switch is incorporated.

Amy Buchmann
Tulane University
abuchman@tulane.edu

MS20

Modeling Hormone Regulation to Examine the Effects of Insulin-Mediated Testosterone Production on Ovulatory Function

Reproductive hormones belong to a tightly regulated system of feedback between the brain and ovaries. Cross-talk between different hormones set the stage for the oscillatory behavior characteristic of the menstrual cycle. In the case of polycystic ovary syndrome (PCOS), a common cause of

infertility, increased ovarian androgen production can disrupt the cycle. Further, elevated insulin is an important cause of the change in androgens. We discuss a mathematical model of the ovulatory cycle and mechanisms of ovarian testosterone production, and we explore ovulatory dysfunction under pathological circumstances, i.e. insulin-dependent changes in testosterone. Model results suggest that variations signal responses of ovarian follicles can alter the extent of ovulatory disruption via elevated insulin. The model also provides insight into the various PCOS phenotypes and the severity of ovulatory dysfunction.

Erica J. Graham
Bryn Mawr College
ejgraham@brynmawr.edu

James F. Selgrade
Department of Mathematics and Biomathematics
Program
selgrade@math.ncsu.edu

MS20
Dna Topology: An Application of Knot Theory to Biochemistry

Although knots have been used since the dawn of humanity, the mathematical study of knots is only a little over 100 years old. Not only has knot theory grown theoretically, the fields of physics, chemistry and molecular biology have provided many applications of mathematical knots. In this talk, I provide an overview of some connections between knot theory and DNA-protein interaction, outlining specifics of the biological mechanisms of DNA replication while providing an overview of related knot invariants.

Candice Price
University of San Diego
cprice@sandiego.edu

MS20
The Effects of Risk Perceptions on An Sis Model

During an outbreak of an infectious disease, uninfected individuals often modify their behavior and are either attracted to, or repelled from, locations based on the perceived risks of infection at each location. Such perceived risks do not necessarily depend on the actual transmission rate or number of infected individuals, but rather on public perception of risk. These dynamics were illustrated with the 2014 Ebola outbreak. In this paper we use a two-dimensional reaction-diffusion-advection model to simulate the dynamics of perceived risks.

Kamuela Yong
University of Hawai?i - West O?ahu
kamuela.yong@hawaii.edu

MS21
Clustered Particle Filtering for High-Dimensional Non-Gaussian Systems

Particle filtering is an essential tool to improve uncertain model predictions by incorporating noisy observational data from complex systems including non-Gaussian features. A new class of particle filters, clustered particle filters, is introduced for high-dimensional nonlinear systems, which uses relatively few particles compared to the standard particle filter. The clustered particle filter captures non-Gaussian features of the true signal which are typical in complex nonlinear dynamical systems such as geophysical systems. The method is also robust in the difficult regime of high-quality sparse and infrequent observations. The key features of the clustered particle filtering are coarse-grained localization through the clustering of the state variables and particle adjustment to stabilize the method. The clustered particle filter is tested for the 40-dimensional Lorenz 96 model with several dynamical regimes including strongly non-Gaussian statistics. The clustered particle filter shows robust skill in both achieving accurate filter results and capturing non-Gaussian statistics of the true signal. It is further extended to multiscale data assimilation, which provides the large-scale estimation by combining a cheap reduced-order forecast model and mixed observations of the large- and small-scale variables. The multiscale clustered particle filter is tested for one-dimensional dispersive wave turbulence using a forecast model with model errors.

Yoonsang Lee
Courant Institute of Mathematical Sciences
New York Univers
ylee@cims.nyu.edu

Majda Andrew
Courant Institute
jonjon@cims.nyu.edu

MS21
Coherent Structure Approaches for Lagrangian Data Assimilation

We introduce a Lagrangian data assimilation method to estimate model parameters by directly assimilating Lagrangian Coherent Structures, where they exist. Our numerical approach is based on the Approximate Bayesian Computation (ABC) framework; however we consider and advocate for a more general methodology, in which coherent structures are considered as reduction tools. We solve the ABC by a Sequential Monte Carlo (SMC) method, and use Principle Component Analysis (PCA) to identify the coherent patterns from tracer trajectory data. Our new method shows remarkably improved results compared to the bootstrap particle filter when the number of (passive) tracers is large, the dynamical system is noisy and the observations are highly informative (i.e. there is small variance in observational error statistics).

John Maclean
University of North Carolina
jhj.maclean@gmail.com

Chris Jones
University of North Carolina-Chapel Hill
ckrtj@email.unc.edu

Naratip Santitissadeekorn
University of Surrey
n/a

MS21
What the Collapse of the Ensemble Kalman Filter Can Tell Us About Localization of Particle Filters

The ensemble Kalman filter (EnKF) is a reliable data assimilation tool for high-dimensional meteorological problems. On the other hand, the EnKF can be interpreted as a particle filter, and particle filters collapse in high-

dimensional problems. We explain that these seemingly contradictory statements offer insights about how particle filters function in certain high-dimensional problems, and in particular support recent efforts in meteorology to "localize' particle filters, i.e., to restrict the influence of an observation to its neighborhood.

Matthias Morzfeld
University of Arizona
Department of Mathematics
mmo@math.arizona.edu

Chris Snyder
Mesoscale and Microscale Meteorology Division
NCAR
chriss@ucar.edu

Daniel Hodyss
Naval Research Laboratory
daniel.hodyss@nrlmry.navy.mil

MS21
Importance Sampling and Data Assimilation

Importance sampling is a building block of many algorithms, perhaps most notably particle filters. It is the importance sampling step that often limits the accuracy of these algorithms. In this talk I will introduce a new way of understanding importance sampling based on information theory. I will argue that the fundamental problem facing algorithms based on importance sampling can be understood in terms of the distance between certain measures. The results give new understanding on the potential use of importance sampling and particle filters in high (possibly infinite) dimensional spaces, as those arising in geophysical applications.

Daniel Sanz-Alonso
Brown University
daniel_sanz-alonso1@brown.edu

MS22
On Efficient Algorithms for Fractional PDEs Arising from Image Restoration and Co-Registration Models

Abstract Not Available At Time Of Publication.

Ke Chen
University of Liverpool
k.chen@liverpool.ac.uk

MS22
Perturbation Theory for Fractional Differential Equations

Regular as well as singular perturbation theory, even for ordinary fractional differential equations seem to be largely missing to date. A perturbative approach, in general coupled to numerical methods, should represent a desirable tool to extract practical information from fractional differential equations. In this talk, we present some results in this direction.

Renato Spigler
Dipartimento di Matematica, Universita Roma tre.
Rome (Italy)
spigler@mat.uniroma3.it

MS22
Fast Numerical Methods for Space-Time Fractional PDEs

Abstract Not Available At Time Of Publication.

Hong Wang
University of South Carolina
Department of Mathematics
hwang@math.sc.edu

MS22
Numerical Methods for Stochastic FPDEs Subject to Uncertain Orders and Random Noise

Abstract Not Available At Time Of Publication.

Mohsen Zayernouri
College of Engineering
Michigan State University
zayern@msu.edu

MS23
Diffusion Geometry and Manifold Learning on Fibre Bundles

A graph synchronization problem over a group searches for an assignment of group elements to the vertices of the graph, such that the two group elements on any two vertices connected by an edge satisfies a compatibility constraint specified by another group element prescribed on that edge. In this talk, we relate synchronization problems on any fixed graph Γ over group G to the moduli space of flat principal G-bundles on Γ, i.e. the G-representation variety of the fundamental group of Γ (viewed as a topological space). This fibre bundle formulation lends itself naturally to many statistical learning problems where information needs to be inferred from only pairwise comparisons of a collection of object data. As a concrete example, we propose *Horizontal Diffusion Maps* — a generalized diffusion geometry framework in the context of manifold learning — that models a dataset with pairwise structural correspondences as a fibre bundle equipped with a connection. We demonstrate the efficacy of this framework in real biological shape classification problems in evolutionary anthropology.

Tingran Gao
Department of Mathematics
Duke University
trgao10@math.duke.edu

MS23
A Variational Approach to Consistency of Graph-Based Methods for Data Clustering and Dimensionality Reduction

When one considers a data cloud embedded in Euclidean space one can endow it with a weighted graph structure in an attempt to leverage the geometry of the ground-truth distribution generating it; the weighted graph can be constructed by giving large weights to pairs of points that are close to each other and the resulting graph can be used for the purposes of data clustering and dimensionality reduction. Algorithms like total variation clustering, spectral clustering, and the mean shift algorithm are examples of graph-based methods for clustering. One can divide these

approaches into those where one seeks to minimize a functional of some sort and those where the clustering is obtained by letting a system evolve over time until a stable state has been reached. Whether it is a minimization problem or it is a system with a gradient flow structure describing the algorithm, it is important to establish consistency results (as the number of observations goes to infinity) for the algorithms and obtain, if possible, convergence rates towards the limiting procedure. In this talk I will present a body of work where strong consistency results are obtained by combining ideas from optimal transportation, calculus of variation, and probability theory.

Nicolas Garcia Trillos
Carnegie Mellon University
nicolas_garcia_trillos@brown.edu

MS23
Sheaves of Probability Distributions

Abstract Not Available At Time Of Publication.

Sanjeevi Krishnan
Ohio State University
sanjeevi@math.osu.edu

MS23
Synchronization over Cartan Motion Groups Via Contraction

The mathematical problem of group synchronization deals with the question of how to estimate unknown set of group elements from a set of their mutual relations. This problem appears as an important step in solving many real world problem such as Structure from Motion (SfM) in vision or pose graph optimization (estimating positions and orientations of mobile robots) in robotics. In this talk, we present a novel solution for synchronization over the class of the non-compact Cartan motion groups, which includes the special important case of rigid motions. Our method is based upon the idea of group contraction, which is a compactification process origin in relativistic mechanics. We show the construction of such a solution for synchronization, analyze some of its theoretical aspects, and illustrate numerically its advantages compared to some current state-of-the-art synchronization methods on both synthetic and real data.

Onur Ozyesil
Princeton
oozyesil@princeton.edu

Nir Sharon, Amit Singer
Princeton University
nsharon@math.princeton.edu, amits@math.princeton.edu

MS24
Gleaming Insights from Analytics on High Throughput Molecular Simulation Data

Thermodynamic data is essential for the design and optimization of chemical engineering processes. Typically, the chemical industry is relying on experimental data. However, this undertaking may be difficult and expensive to conduct or even practically impossible, especially in the case of hazardous substances. An alternative route is available through molecular modelling and simulation on the basis of classical force fields. Along with its powerful predictive capabilities, it allows for large datasets of thermophysical data to be produced with considerably less effort than laboratory measurements. However, setting up molecular simulations and interpreting simulation data requires expertise. This presentation will focus on designing automized data analytics approaches to provide insights based on high throughput molecular simulation data.

Colin W. Glass
High Performance Computing Center Stuttgart, Germany
glass@hlrs.de

MS24
HPC and Data Science in Molecular Engineering: An Overview on Molecular and Multiscale Simulation and Analysis

The importance of molecular modeling and simulation for engineering applications increases rapidly due to improvements in the numerical accuracy and the accessible length and time scales. Reaching quantitative agreement with the available data, and predicting properties where experimental data are absent, molecular engineering transforms engineering data science. The major challenge today consists in integrating various levels, including molecular simulation codes, reliable molecular models, equations of state, mesoscopic methods, property databases, and process models, to a coherent framework. Accordingly, the opening statement for the minisymposium on HPC and Data Science in Molecular Engineering will review the state of the art, discuss the tendencies of development which are already present, and sketch promising directions for future work and future discussions. In particular, results will be reviewed which were obtained from recent work using the MD program ls1 mardyn and the macro-micro-coupling tool for molecular-continuum simulations.

Martin T. Horsch
University of Kaiserslautern, Germany
Laboratory of Engineering Thermodynamics
martin.horsch@mv.uni-kl.de

Philipp Neumann
University of Hamburg, Germany
Scientific Computing
philipp.neumann@uni-hamburg.de

MS24
Large-Scale Molecular Dynamics Simulations at the Argonne Leadership Computing Facility

In this talk we will describe multiple aspects of running large-scale molecular dynamics simulations at the Argonne Leadership Computing Facility (ALCF). We will start by describing the ALCF, its mission to accelerate major scientific discoveries and engineering breakthroughs for humanity, and operating some of the most powerful supercomputers on the planet to help researchers solve some of the worlds largest and most complex problems. We will cover some of the molecular dynamics scientific codes used at ALCF, along with science results from recent large-scale simulations. In addition, we will also touch on large-scale visualization and analysis to enable scientific discovery from molecular dynamics simulations, as well as the challenges in transitioning to the in-situ paradigm. To conclude, we will present an overview of molecular dynamics simulations on upcoming many-core supercomputer archi-

tectures.

Silvio Rizzi
Argonne National Laboratory
Leadership Computing Facility
srizzi@anl.gov

Joseph Insley
Argonne National Laboratory
insley@anl.gov

MS24

Simulating Human Red Blood Cells at Protein Resolution with the Openrbc Molecular Dynamics Package

OpenRBC is our latest development of a coarse-grained molecular dynamics code, which is capable of performing an unprecedented in silico experiment — simulating an entire mammal red blood cell lipid bilayer and cytoskeleton modeled by millions mesoscopic particles — on a single shared memory node. To achieve this, we invented an adaptive spatial searching algorithm to accelerate the computation of short-range pairwise interactions in an extremely sparse 3D space. The algorithm is based on a Voronoi partitioning of the point cloud of coarse-grained particles, and is continuously updated over the course of the simulation. The algorithm enables the construction of a lattice-free cell list, i.e. the key spatial searching data structure in our code, in $O(N)$ time and space with cells whose position and shape adapts automatically to the local density and curvature. The code implements NUMA/NUCA-aware OpenMP parallelization and achieves ideal scaling with hundreds of hardware threads. It outperforms a legacy solver by an order of magnitude in time-to-solution and two orders of magnitude in problem size, thus providing a new venue for probing the biomechanics of red blood cells.

Yu-Hang Tang, Lu Lu, He Li
Brown University
yuhang_tang@brown.edu, lu_lu_1@brown.edu,
he_li@brown.edu

Constantinos Evangelinos
Computational Science Center
IBM T.J. Watson Research
cevange@us.ibm.com

Leopold Grinberg
IBM Corporation
leopoldgrinberg@us.ibm.com

Vipin Sachdeva
IBM T. J. Watson Research Center, Cambridge, MA
IBM
vsachde@us.ibm.com

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS25

Measuring Conductivity and Validation Using Current Density Imaging

A new non-invasive validation procedure has been devel-oped to assess the accuracy of any conductivity imaging method. This procedure is based on a testing current measured using Current Density Imaging (CDI), a method pioneered by Scott, Joy, Armstrong and Henkelman to determine applied currents in tissue using a Magnetic Resonance Imager. The ability of the proposed procedure to quantify the dependence of the accuracy of the conductivity reconstruction methods on the level of anisotropy was studied on a carefully simulated data for a finite element model of realistic brain tissue, for which we have the ability to tune the level of anisotropy. Tests were carried out for three different levels of tissue anisotropy to compare the results obtained by our recently developed anisotropic conductivity imaging method Diffusion Tensor Current Density Impedance Imaging (DT-CD-II) with those obtained by the well-established Current Density Impedance Imaging (CDII) method that assumes the conductivity to be isotropic. The results show that the conductivity imaging method which takes into account tissue anisotropy yields significantly superior accuracy even for conductivities with a low level of fractional anisotropy. The validation procedure was also shown to be applicable to a third, and different conductivity imaging method (MCDII) proposed by Nachman, Tamasan and Timonov, that requires only the magnitude of one current and the corresponding boundary voltage.

Nahla M. Elsaid
University of Maryland
nahola@gmail.com

Adrian Nachman
University of Toronto
nachman@math.toronto.edu

Weijing Ma
Faculty of Applied Science and Technologies
Sheridan College
weijing.ma@sheridancollege.ca

Michael Joy
University of Toronto
mike.joy@utoronto.ca

MS25

Problems in Electromagnetic Imaging

We describe problems that arise in attempting to image the electromagnetic properties inside a body from measurements made on the surface of that body. At low frequencies this is mathematically equivalent to the Calderon Problem of Electrical Impedance Tomography (EIT). We show how the desire to maximize the differences in measurements between internal states, such as the heart filled with blood , and the heart depleted of blood, led to the design of Adaptive Current Tomography (ACT) systems. At higher frequencies we are led to optimization and inverse problems for the Maxwell, and Maxwell Bloch systems of equations. It will be explained how the desire to image the internal conductivity, permittivity, permeability, spin densities, and relaxation times , leads to additional mathematical problems in the design of electromagnetic imaging systems.

David Isaacson
RPI

isaacd@rpi.edu

MS25

Stroke Classification and Monitoring Using Electrical Impedance Tomography

Stroke is one of the leading causes of death in the world. There are two main types of stroke: ischemic, due to lack of blood flow, and hemorrhagic, due to bleeding. During every hour of untreated ischemic stroke, the brain loses as many neurons as it does in several years of normal aging. Unfortunately, ischemic and hemorrhagic strokes have exactly the same symptoms, and classification of these two kinds of stroke can only be done by brain imaging using MRI or CT at large hospitals. In this talk, we introduce the so-called CGO-Fourier method for stroke detection. This approach is an extension of the D-bar method, and is the first EIT algorithm that is designed to see through layers such as the resistive skull. Numerical results for simulated strokes in 2D and 3D cases show that this approach is an promising imaging technique that allows to instantly classify stroke in the ambulance.

Minh N. Mach
University of Helsinki
minh.mach@helsinki.fi

Samuli Siltanen, Andreas Hauptmann
University of Helsinki
Finland
samuli.siltanen@helsinki.fi, andreas.hauptmann@helsinki.fi

MS25

Recent Development in Anisotropic Electrical Impedance Tomography Using Bayesian Framework

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 wide variety of applications including medical imaging and geophysical prospecting. This talk presents a Bayesian approach to the estimation of an anisotropic conductivity from EIT data. We present the inner and outer iteration scheme for computing a maximum *a posteriori* estimate, and show results from simulated data.

Rashmi Murthy
Department of Mathematics
Colorado State University
murthy@math.colostate.edu

Jennifer L. Mueller
Colorado State University
Dept of Mathematics
jennifer.l.mueller@gmail.com

MS26

The Dynamic Consequences of Evolution in Response to Environmental Disturbances

Prolonged exposure to a disturbance such as a toxicant has the potential to result in rapid evolution of toxicant toler-ance in many short-lived species. This evolution may allow a population to persist at higher levels of the toxicant than is possible without evolution. Here we apply evolutionary game theory to Leslie matrix models to obtain Darwinian equations that couple population and evolutionary dynamics. We use these models to consider how the evolution of tolerance to a disturbance may change the population dynamics of both the focal population and interacting populations. We provide an application to Daphnia and determine the conditions under which a Daphnia population can persist by evolving toxicant tolerance. We then extend this idea to a predator-prey system in which the prey evolves in response to a toxicant but the predator does not due to different time scales. We consider how evolution in the prey species impacts the population dynamics of the predator species. This model is inspired by marine mammals which have significantly longer lifespans relative to their food sources.

Azmy S. Ackleh
Department of Mathematics
University of Louisiana at Lafayette
ackleh@louisiana.edu

MS26

Modeling Bumble Bee Population Dynamics with Delay Differential Equations

Bumble bee populations have been decreasing in recent decades, with demise of flower resources and pesticide exposure being two of several suggested pressures causing declines. To provide a tool for projecting and testing sensitivity of growth of populations under contrasting and combined pressures, we developed a non-linear, non-autonomous delay differential equation (DDE) model of bumblebee colonies and resources. We explain the usefulness of delay equations as a natural modeling formulation, particularly for bumble bee modeling. We introduce a specific numerical method that approximates the solution of the delay model and investigate conditions to assure convergent approximate solutions. We also describe ways in which resource limitation, pesticide exposure and other pressures can be reflected in the model. The efforts represent collaborations between our group at NCSU and ecologists at California State University, Monterey Bay and the Swedish University of Agricultural Sciences, Uppsala.

H. T. Banks
NC State University
Center for Research in Scientific Computation
htbanks@ncsu.edu

MS26

A Periodically Forced Matrix Model for the Dynamics of a Seasonally Reproducing Population

I will describe a discrete time, structured population dynamics model designed to explain some observed phenomena in marine bird colonies by our research team (on Protection Island National Wildlife Refuge). The model extends earlier models for the population dynamics during breeding seasons by means of an across-season map (during which maturation occurs). Mathematically, the model is a periodically forced semi-dynamical system which, by means of a dimensional reduction applied to the composite map, is subject to a significant amount of analysis. I will present some results of the analysis which focus on model predicted extinction vs. persistence. I will also present other results which have ecological implications that relate

environmental degradation to population survival and to observed behavioral changes (e.g. cannibalism and reproductive synchrony).

Jim M. Cushing
Department of Mathematics
University of Arizona
cushing@math.arizona.edu

MS26

Backward Bifurcation and Oscillations in a Nested Immuno-Eco-Epidemiological Model

This talk introduces a novel partial differential equation immuno-eco- epidemiological model of competition where species 1 is affected by a disease while species 2 can compete by lowering species 1 immune response to the infection, a mode of competition termed stress-induced competition. When the disease is chronic, we reduce the partial differential equation model to a three dimensional ordinary differ- ential equation model. The ODE model exhibits backward bifurcation and sustained oscillations caused by the stress-induced competition. Furthermore, the ODE model, although not a special case of the PDE model, guides effectively in detecting back- ward bifurcation and oscillations in the PDE model. Stress-induced competition re- lated backward bifurcation allows species 2 to persist for values of its invasion number below one. Furthermore, stress-induced competition leads to destabilization of the co- existence equilibrium and sustained oscillations in the PDE model. We suggest that complex systems such as this one may be studied by appropriately designed simple ODE models.

Maia Martcheva, Michael Barfield
University of Florida
maia@ufl.edu, mjb01@ufl.edu

Necibe Tuncer
Florida Atlantic University
ntuncer@fau.edu

Robert Holt
University of Florida
rdholt@ufl.edu

MS27

Analysis of Market Stability Through Experiments, Statistical Studies and Mathematical Modeling

Stability is of crucial importance in asset markets. Classical theories do not address abrupt changes in the price in the absence of fundamental changes, labeling them anomalies or rare but possible events in a stochastic system. Behavioral finance researchers believe, however, that such events can be attributed to motivations of traders beyond those generated by valuation. Thus, one approach to this issue is through an examination of additional motivations such as trend following, or momentum. In a more general context, this is the effect of sentiment. This talk will focus on deriving the importance of trends in terms of experimental and statistical large data studies and analysis through systems of differential equations. In particular, the laboratory bubbles experiments demonstrate the role of cash/asset ratio and momentum trading. The statistical studies show that price trend has a nonlinear effect. The Asset Flow Differential Equations (AFDE) can be used to study stability in the sense of dynamical systems. In particular, the AFDE show that as more traders utilize mo-

mentum trading and with a shorter time scale, markets tend to be less stable.

Gunduz Caginalp
University of Pittsburgh
Department of Mathematics
caginalp@pitt.edu

MS27

Slow-Fast Analysis of a Multi-Group Asset Flow Model with Implications for the Dynamics of Wealth

The multi-group asset flow model is a nonlinear dynamical system developed as a tool for understanding the behavioral foundations of market phenomena such as flash crashes and price bubbles. We use that model to analyze the dynamics of the market when investors' trading rates (i.e., their desire to exchange stock for cash) are prescribed ahead of time independently of the state of the market. We decompose the dynamics of the system to fast and slow components. We show that the dynamics of the slow system is rate-invariant, i.e., the state of the system depends on the path of the input trading rates in rate space, but not the time of travel along the path. We also find that the slow system is not integrable in the sense that cyclic trading rate paths do not return the system to the initial state. We use these mathematical results to derive a variety of observations regarding the dynamics of investors' wealth. In particular, we show that strategies with constant trading rates, which represent the well-known constant-rebalanced portfolio (CRP) strategies, are optimal in the sense that they minimize investment risks as they preserve the investor's wealth after any cycle in which the price of the asset returns to its starting value. In contrast, any cyclic non-CRP strategy can be exploited by another, appropriately defined, cyclic non-CRP strategy in a predatory trading process, i.e., a process in which one investor achieves gains in wealth at the expense of another investor.

Mark DeSantis
Argyros School of Business and Economics
Chapman University
desantis@chapman.edu

MS27

Bifurcation Analysis of a Single Group Asset Flow Model

The stability and Hopf bifurcation analysis of an asset pricing model under the assumption of a fixed amount of cash and stock in the system will be presented. The model analyzed is based on the model introduced by Caginalp and Balenovich and consists of a system of the Asset Flow Differential Equations (AFDE) that can be used to study stability in the sense of dynamical systems. First, we analyze stability of equilibrium points. Choosing the momentum coefficient as a bifurcation parameter, we also show that Hopf bifurcation occurs when the bifurcation parameter passes through a critical value. Analytical results are supported by numerical simulations. A key conclusion for economics and finance is the existence of periodic solutions in the absence of exogenous factors for an interval of the bifurcation parameter, which is the trend-based (or momentum) coefficient.

Huseyin Merdan
TOBB Univ of Economics and Technology
Ankara, Turkey

merdan@etu.edu.tr

MS27
Investor Sentiment in the Stock Market

Abstract Not Available At Time Of Publication.

Jeffrey Wurgler
Stern
New York University
jwurgler@stern.nyu.edu

MS28
Correcting the Biasedness of the Value-at-Risk and Conditional Tail Expectation

Stocks and Options are investment instruments. Investments are prone to the risk of losses caused by, for example, market risk. This risk need to be measured so that investors may be able to make plans to mitigate a loss. In practice, the variance of returns is often used to measure investment risk. However, in order to manage investment risks more appropriately, other risks measures are needed. This final project discusses two risk measures, namely the Value-at-Risk (VaR) and the Conditional Tail Expectation (CTE). These risk measures require the calculation of the quaniles of a loss distribution. VaR is defined as the maximum loss that can be tolerated to a certain level of significance. CTE measures losses in terms of the expectation of the excess of a VaR. In this final project, a number of estimators for the VaR and CTE are discussed. The biasedness of such estimators are measured and corrected. The Monte Carlo simulation and the Bootstrap method are used to measure the biasedness. Biased-corrected estimators are then applied to estimate the VaR and the CTE of the loss distribution of the returns of an investment on a particular stock.

Nuzulia Fajri Rahmi, Dumaria R. Tampubolon
Institut Teknologi Bandung
Lia.affandi@students.itb.ac.id, dumaria@math.itb.ac.id

MS28
Prediction of Valuable Customers

Nowadays companies gather a huge amount of data about their customers. This data can provide meaningful insights which can improve business as well as customer experience and satisfaction. In this paper we apply machine learning techniques to identify customers who have the most potential business value for the company. This is done based on the customer's characteristics and activities. The certain patterns in the activities provide us major insights on improving business. This way companies can effectively prioritize resources to the right customers. We tested our model during Kaggle-based Predicting Red Hat Business Value 2016.

Chirag Girdhar, Janpreet Singh
Indian Institute of Technology(Indian School Of Mines)
chiraggirdhar95@gmail.com , janpreetsingh.1@gmail.com

MS28
Relaxation in BH of Second Order Structured Deformations

In the theory of continuum mechanics, it is often the case that the macroscopic deformation field does not accurately describe sub-macroscopic changes in geometry. Disagreements between the macroscopic and microscopic description correspond to the onset of defects in the microstructrue. This is the basis of the theory of structured deformations. In order to account for so-called "gradient disarrangements", one must extend this theory up to second order, the appropriate underlying function space being the space BH of Bounded Hessian. We apply blow-up techniques to obtain an integral representation for the relaxation of energy functionals in BH with an additional microscopic description.

Adrian Hagerty
Carnegie Mellon University
achagerty@gmail.com

MS28
Simulation of Phase Transitions in Gene-gene Interaction Networks

A key aim of biomedical research is to systematically catalogue all genes and their interactions within a living cell. The commonly adopted approach to study such complex interacting systems, reductionism, has dominated biological research and has given in depth insights about individual cellular components and their functions. However it is increasingly clear that formulations where a single biological function attributed to an individual component is not accurate since most biological characteristics arise from strong interaction of biological entities in complex networks leading to unexpected biological responses on local modes of action. Here I present a new approach, at the intersection of network biology and statistical mechanics, a study of the effect of local perturbations (e.g. loss of gene expression) on the phase transition profiles of an Ising model network with sensitivity analysis of real-life data. The effects of stress is modeled as external noise that could be locally weak, but broadly distributed on the network (like environmental stress in fermentations of plants) or stress that are locally strong but duration of application short (adverse drug effects) leading to irreversible phase transition. The evolution of Ising states of network show critical points of phase transitions in analogy to thermodynamics.

Jeyashree Krishnan
Aachen Institute for advanced study in Computational Enginee
RWTH Aachen University
krishnan@aices.rwth-aachen.de

MS28
A Sharp Interface Model and its Numerical Approximation of Solid-state Dewetting in Three Dimensions

Solid thin films on substrate are typically unstable and can exhibit complicated morphologies evolution even below their melting temperature. Driven by capillary instabilities, the thin film can produce a series of growing holes, retracting edges, or even break up into small islands. This process, known as dewetting, tends to minimize the total surface energies of the system via surface diffusion while preserve the volume of the thin film. So based on the thermodynamic variation, we derive the sharp interface model of solid-state dewetting on a flat substrate. The governing equations for the problem belongs to the 4-th order geometric partial differential equations which include the surface diffusion flow and contact line migrations. We then propose a varitional formulation for the sharp interface model

and apply parametric finite element method to solve it.

Zhao Quan
National University of Singapore
A0109999@u.nus.edu

Bao Weizhu
National University of Singapore
Department of Mathematics
matbao@nus.edu.sg

Wei Jiang
National University of Singapore and Wuhan University
jiangwei1007@whu.edu.cn

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS28
PDE Constrained Optimization with Multiscale Methods

PDE parameter estimation problems arise frequently in many applications such as geophysical and medical imaging. Commonly, the inverse problem is formulated as an optimization problem whose constraints are given by the underlying PDEs. We consider the so-called reduced formulation in which the PDEs are eliminated. The resulting unconstrained optimization problem is computationally expensive to solve because they require solving the underlying PDEs numerous times until the reconstruction of the parameter is sufficiently accurate. We consider the case in which many measurements are available leading to a large number of PDE constraints. To reduce the costs of the PDE solvers, we discuss multiscale reduced order modeling (ROM) scheme that projects the discretized forward problems onto a lower dimensional subspace. This is done through an operator-induced interpolation by solving PDEs locally on coarse cells. By design, this interpolation accounts for the parameter changes and thus the basis adapts to the current estimate of the parameters. We outline an optimization method that includes the derivatives of the adaptive multiscale basis. We demonstrate the potential of the method using examples from geophysical imaging.

Samy Wu Fung
Emory University
400 Dowman Dr, 30322 Atlanta, GA, USA
samy.wu@emory.edu

MS29
Pattern Formation in Networks of (Nonsmooth) Firing Equations

We study the activity of coupled populations of excitatory and inhibitory neurons in a neural firing rate model that includes 1D nonlocal, spatial coupling. To facilitate analysis of traveling waves, we approximate the (typically smooth) nonlinear firing rate function with the Heaviside step function. We study the corresponding nonsmooth differential system in traveling wave coordinates, with a particular interest in how the system transitions from a traveling front to pulse as the temporal and spatial scales of inhibition vary.

Jeremy D. Harris
Department of Mathematics
University of Pittsburgh
jdh71@pitt.edu

Bard Ermentrout
University of Pittsburgh
Department of Mathematics
bard@pitt.edu

MS29
Emergent Dynamics from Network Connectivity: A Minimal Model

Even in the absence of changing sensory inputs, many networks in the brain exhibit *emergent dynamics* – that is patterns of activity that are shaped by the intrinsic structure of the network rather than modulated by an external input. Such dynamics are believed to underlie central pattern generators (CPGs) for locomotion, oscillatory activity in both hippocampus and cortex, and the complex interplay between sensory-driven responses and ongoing spontaneous activity. To isolate the role of network connectivity alone in shaping these dynamics, we introduce the *Combinatorial Threshold Linear Network* (CTLN) model, a minimal model with binary synapses, simple perceptron-like neurons, and flat external input, whose dynamics are controlled solely by the structure of an underlying directed graph. The simple piecewise linear activation function for the neurons is sufficient to produce the full variety of nonlinear dynamics: multistability, limit cycles, chaos, and even quasiperiodic behavior. By varying only the underlying graph, we observe emergent dynamics relevant for computational functions in cortex, hippocampus and CPGs: multistability, fast sequences, slower "cell assembly" sequences, and complex rhythms. The CTLN model is also highly amenable to mathematical analysis, and we prove theorems characterizing features of the emergent dynamics based on the structure of the underlying graph.

Katherine Morrison
School of Mathematical Sciences
University of Northern Colorado
katherine.morrison@unco.edu

MS29
Phase Response Curves for Limit Cycles in Filippov Systems

The asymptotic phase θ of an initial condition x in the stable manifold of a limit cycle identifies the phase of the point on the limit cycle to which the flow $\phi_t(x)$ converges as $t \to \infty$. The infinitesimal phase response curve (iPRC) quantifies the change in timing due to a small perturbation of a limit cycle trajectory. For a stable limit cycle in a smooth dynamical system the iPRC is the gradient $\nabla_x(\theta)$ of the phase function, which can be obtained via the adjoint of the variational equation. For systems with discontinuous dynamics, the standard approach to obtaining the iPRC fails. We derive a formula for the infinitesimal phase response curves (iPRCs) of limit cycles occurring in piecewise smooth (Filippov) dynamical systems of arbitrary dimension, subject to a transverse flow condition. Discontinuous jumps in the iPRC can occur at the boundaries separating subdomains, and are captured by a linear matching condition. The matching matrix, M, plays a role analogous to the saltation matrix arising in variational problems. For the special case of linear dynamics away from switching boundaries, we obtain an explicit expression for the iPRC. We present examples from cell biology (Glass networks) and neuroscience (central pattern generator models). We

apply the iPRCs obtained to predict synchronization and antisynchronization in a threshold-linear network model.

Youngmin Park
University of Pittsburgh
yop6@pitt.edu

Kendrick Shaw
Case Western Reserve University
Department of Biology
kms15@case.edu

Hillel Chiel, Peter J. Thomas
Case Western Reserve University
hjc@case.edu, pjthomas@case.edu

MS29

Piecewise Smooth Models of a Biological Motor Control System

Motor systems must adapt to perturbations and changing conditions both within and outside the body. We refer to the ability of a system to maintain performance despite perturbations as "robustness, and the ability of a system to deploy alternative strategies that improve fitness as "flexibility. Here we explore how sensory feedback could alter a neuromechanical trajectory to enhance robustness for motor control. The underlying mechanism would be (1) to adjust the timing of a particular phase of the trajectory or (2) to vary the path of neuromechanical trajectories, or (3) to switch between qualitatively distinct trajectory types (robustness through flexibility). As a concrete example, we focus on a piecewise smooth neuromechanical model of triphasic motor patterns in the feeding apparatus of the marine mollusk *Aplasia californica*. To show that sensory feedback robustly alters neuromechanical trajectories, moderate mechanical or neural perturbations are applied to an experimental neuromechanical preparation. We also extend and apply variational techniques (phase response curves, linear approximation) to our neuromechanical system to determine how it maintains robustness in response to such perturbations.

Yangyang Wang
Mathematical Biosciences Institute
The Ohio State University
wang.9737@mbi.osu.edu

Jeff Gill, Hillel Chiel
Department of Biology
Case Western Reserve University
jeff.gill@case.edu, hillel.chiel@case.edu

Peter J. Thomas
Case Western Reserve University
pjthomas@case.edu

MS30

Zeno Breaking, the 'Contact' Effect, and Sensitive Behaviour in Piecewise Linear Systems

Abstract Not Available At Time Of Publication.

Roderick Edwards
University of Victoria
Dept. Math and Statistics
edwards@uvic.ca

MS30

Regularisation of Piecewise Smooth Dynamical Systems, with Application to the Painlev Paradox

Abstract Not Available At Time Of Publication.

John Hogan
Bristol Centre for Applied Nonlinear Mathematics
Department of Engineering Mathematics, University of Bristol
s.j.hogan@bristol.ac.uk

MS30

On Temporal Indeterminacy in Piecewise Smooth Systems

Continuity in a dynamical system is known to not be a sufficient property to guarantee the uniqueness of its solutions. Here we consider piecewise smooth systems where ambiguity arises when the temporal determinacy of a solution is lost. In phase-space this corresponds to the same spatial trajectory being traversed in different times, as the solution pauses arbitrarily long at particular points. This potentially mimics behaviour seen in earthquakes and static friction models, where periods of dynamic activity are separated by seemingly static phases of unpredictable length. We study piecewise smooth systems containing temporal (and sometimes spatial) ambiguities that can be partly resolved through application of parameter rescalings and asymptotic balancing; except at particular parameter values where the uncertainty persists. These are our pausing points. We present examples of the phenomena occurring at a fold-fold singularity in a system drawn from a gene regulation model, and in the impacting system of the classical Painlevé paradox.

Simon C. Webber
University of Bristol
Department of Engineering Mathematics
scwebber.2011@my.bristol.ac.uk

Paul Glendinning
University of Manchester
p.a.glendinning@manchester.ac.uk

Mike R. Jeffrey
University of Bristol
mike.jeffrey@bristol.ac.uk

MS31

Panelists To Be Announced

Abstract Not Available At Time Of Publication.

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MS32

A Bayesian Approach to Value of Information: Exploring the Value of Waiting During a Trial of Labor

Of the nearly 4 million births that occur each year in the United States, almost one in every three is a cesarean de-

livery. With a rate of 32.2% in 2014, the proportion of babies delivered by cesarean section (CS) has steadily increased over the years from an initial recording of 4.5% in 1965. Despite the increase in CS rate, there is no evidence that this increasing rate has caused a decrease in neonatal or maternal mortality or morbidity. I will present two variations of a Bayesian decision model used to determine when to classify a patient as "failure-to-progress' using either current information (prior probability) or information gathered (posterior probability) as labor continues. The Bayesian decision models determine the conditions under which it is appropriate to gather additional information (i.e., take an observation) prior to deciding to end a trial of labor and perform a CS based on the decision maker's belief of a successful trial of labor. The first model assumes labor progression can be modeled by an exponential probability distribution and the second model assumes labor progression is log-normally distributed. This study determines the conditional value of information (conditional on the decision maker's prior belief) and determines the conditions under which information has positive value. This model can be used to facilitate shared decision making through communicating beliefs, risk perceptions, and the associated actions.

Karen T. Hicklin
The University of North Carolina at Chapel Hill
khicklin@email.unc.edu

Julie Ivy, Fay Cobb Payton
North Carolina State University
jsivy@ncsu.edu, fcpayton@ncsu.edu

Meera Viswanathan
RTI International
viswanathan@rti.org

Evan Myers
Duke University School of Medicine
evan.myers@duke.edu

MS32

Hurricane Uncertainty Propagation for Real-Time Storm Surge Forecasting

In recent decades, computational hurricane storm surge models have become increasingly accurate due to improvements in numerical methods, improved model parameters, and implications of advancements in high performance computing, e.g. the ability to more finely resolve model domains. Unfortunately, when storm surges are estimated in real-time, many uncertainties are introduced due to the uncertainties in the hurricane (i.e. wind) forecast itself. To aid in emergency response, an ensemble of hurricane scenarios is used to determine a range of possibilities of storm surge inundation. However, the likelihood of each scenario remains unclear. Here, we use the uncertainties associated with various storm parameters to estimate these likelihoods. We also investigate the evolution of the likelihoods as the uncertainty in the hurricane forecasts is reduced.

Talea Mayo
University of Central Florida
talea.mayo@ucf.edu

MS32

Stochastic Optimization Using Parametric Cost

Function Approximations

A widely used heuristic for solving stochastic optimization problems is to use a deterministic rolling horizon procedure, which has been modified to handle uncertainty (e.g. buffer stocks, schedule slack). We formalize this strategy and call it a parametric cost function approximation where parameterized modifications of costs or constraints can be adaptively learned using the principles of policy search. We will also present stochastic algorithms for tuning the policy in a simulator.

Raymond Perkins
Princeton University
raymondp@princeton.edu

MS33

Accuracy of a Class of Nonlinear Filters for Quasilinear Dynamics in the Presence of Model Error

We consider the filtering problem for estimating quasilinear and quadratic truth dynamics with linear observations where the optimal estimate is given w.r.t. a quadratic cost function. The filter equations are derived by exploiting connections to a dual stochastic control problem. In particular, this approach provides a framework for a systematic derivation of suboptimal Bayesian filters with a systematic update on the error covariance. The two-dimensional, incompressible Navier-Stokes equation in a periodic geometry is utilised to illustrate the results in distinct dynamical regimes with sparse observations aliasing fine-scale information into the assimilation space.

Michal Branicki
University of Edinburgh
m.branicki@ed.ac.uk

MS33

Correcting Biased Observation Model Error in Data Assimilation

While the formulation of most data assimilation schemes assumes an unbiased observation model error, in real applications, model error with nontrivial biases is unavoidable. A practical example is errors in the radiative transfer model (which is used to assimilate satellite measurements) in the presence of clouds. Together with the dynamical model error, many (in fact 99%) of the cloudy observed measurements are not being used although they may contain useful information. I will discuss a novel nonparametric Bayesian scheme which is able to learn the observation model error distribution and correct the bias in incoming observations. This scheme can be used in tandem with any data assimilation forecasting system. The proposed model error estimator uses nonparametric likelihood functions constructed with data-driven basis functions based on the theory of kernel embeddings of conditional distributions developed in the machine learning community. We will show numerical results of assimilating cloudy satellite brightness temperature-like quantities, generated from a stochastic multicloud model for tropical convection and a simple radiative transfer model.

John Harlim
Pennsylvania State University
jharlim@psu.edu

MS33

Analysis of a Nudging-Based Algorithm for Data

Assimilation

The purpose of this talk is to present some analysis results concerning a feedback-control (nudging) approach for data assimilation that works for a general class of dissipative dynamical systems and observables. First, I will consider the situation when the measurements are discrete in time and contaminated by systematic errors. In this case, we obtain an estimate for the error between the approximating solution and the reference solution that shows exponential convergence in time modulo the bound on the errors. Later, I will consider a numerical approximation of the nudging equation via the Postprocessing Galerkin Method, and show an analytical estimate of the truncation error committed in this finite-dimensional approximation. Most importantly, this error estimate is uniform in time. This is in contrast with the error estimate for the usual Galerkin approximation of the 2D Navier-Stokes equations, which grows exponentially in time. This talk is based on joint works with C. Foias and E. S. Titi.

Cecilia F. Mondaini
Texas A&M University
cmondaini@math.tamu.edu

Ciprian Foias
Texas A & M,
Indiana University
foias@math.tamu.edu

Edriss S. Titi
Texas A&M University
Weizmann Institute of Science
titi@math.tamu.edu, edriss.titi@weizmann.ac.il

MS33
Projected Data Assimilation

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.

Erik Van Vleck
University of Kansas
erikvv@ku.edu

MS34
Modeling and Simulation for Tempered Anomalous Dynamics

Abstract Not Available At Time Of Publication.

Weihua Deng
Department of Mathematics
Lanzhou University, China
dengwh@lzu.edu.cn

MS34
Principal Orthogonal Decomposition for Fractional Differential Equations

Fractional differential equations (FDEs) have recently been used to model phenomena with long-range interactions and memory effects, including diffusion in fractured media, constitutive laws for viscoelastic materials, and sediment transport in riverbeds. Because FDEs involve non-local operators, existing numerical methods typically require a great deal of computational cost and storage to discretize and solve these equations. While conventional spectral methods for solving FDEs require a high number of basis modes to approximate the solution with a sufficiently small error, the manifold in which the solution actually resides may well be spanned by a small number of modes if they are chosen correctly. Proper Orthogonal Decomposition (POD) has been used in the context of integer-order differential equations to reduce the number of basis functions needed to represent the solution. In this talk, we will demonstrate how we can use POD to construct a basis specially suited to our fractional equations that will enable us to find a low-dimensional approximation to the solution, producing a more efficient solver. We will demonstrate the accuracy and efficiency of this technique with numerical examples.

Anna Lischke
Brown University
anna_lischke@brown.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS34

A Petro-Galerkin Method of Linear Complexity and Exponential Convergence for the 1-D Diffusion Equation with Two-Sided Fractional Derivatives

An open problem in the numerical solution of fractional partial differential equations (FPDEs) is how to obtain high-order accuracy for singular solutions; even for smooth right-hand-sides solutions of FPDEs are singular. Here, we consider the 1-D diffusion equation with general two-sided fractional derivative characterized by a parameter $p \in [0, 1]$; for $p = 1/2$ we recover the Riesz fractional derivative while for $p = 1, 0$ we obtain the one-sided fractional derivative. We employ a Petrov-Galerkin projection in a properly weighted Sobolev space with (two-sided) Jacobi polyfracnomials as basis and test functions. In particular, we derive these two-sided Jacobi polyfractonomials as eigenfunctions of a Sturm-Liouville problem with weights uniquely determined by the parameter p. We provide a rigorous analysis and obtain optimal error estimates that depend on the regularity of the forcing term, i.e., for smooth data (corresponding to singular solutions) we obtain exponential convergence while for smooth solutions we obtain algebraic convergence. We demonstrate the sharpness of our error estimates with numerical examples, and we present comparisons with a competitive spectral collocation method of tunable accuracy. We also investigate numerically deviations from the theory for inhomogeneous Dirichlet boundary conditions as well as for a fractional diffusion-reaction equation.

Zhiping Mao
Brown University, USA
zhiping_mao@brown.edu

George Em Karniadakis
Brown University

george_karniadakis@brown.edu

MS34
A Universal Fractional Model for Wall Turbulence

Currently there is no universal descriptions of the mean velocity profile in wall turbulent flows that is valid for all Reynolds numbers. The objective of this paper is to use non-local modeling via fractional PDEs to develop predictive models for the mean velocity profile, from the wall all the way to the freestream. We consider a variable fractional order differential equation to govern the mean turbulent flow since the small-scale components can be described as anomalous diffusion. Using model inversion techniques and data from Direct Numerical Simulations (DNS) up to viscous Reynolds number 5,000 we extract the functional form of the fractional order, which if scaled appropriately shows universality. We then use this universal law and solved a simple fractional PDE to obtain velocity profiles in fully-developed flow channels and pipes, including the Princeton superpipe, at viscous Reynolds numbers up to 100,000.

Fangying Song
Division of Applied Mathematics
Brown University
fangying_song@brown.edu

George Em Karniadakis
Brown University
george_karniadakis@brown.edu

MS35
Multiscale Fast Algorithm for STORM Imaging

Stochastic optical reconstruction microscopy (STORM) is a widely used single-molecule-based super-resolution light microscopy methods. In biological research, numerous breakthroughs have been enabled by this imaging modality. Multiscale Fast Algorithm for STORM Imaging proposes a multiscale algorithm to accelerate processing STROM images. It is a novel work for efficient reconstruction of biomedical images. This algorithm is capable to accurately identify the true particle locations from overlapping diffraction patterns. Therefore, the overall reconstruction can be processed within a small amount of STORM images, which, in turn, enables the live video of a cell. Numerical experiments demonstrate the accuracy and efficiency of the new algorithm.

Yingzhou Li
Stanford
ryanli@stanford.edu

MS35
On the Convergence of Recursive Schemes for Wave Shape Functions

This talk is about a novel recursive diffeomorphism based scheme for one-dimensional generalized mode decomposition problem that aims at extracting generalized modes $\alpha_k(t)s_k(2\pi N_k\phi_k(t))$ from their superposition $\sum_{k=1}^{K}\alpha_k(t)s_k(2\pi N_k\phi_k(t))$, assuming that amplitude and phase functions $\alpha_k(t)$ and $N_k\phi_k(t)$ are known. We introduce a few newly developed approaches to estimate wave shape functions $s_k(t)$ and prove the convergence of the recursive scheme. If time permitted, a fast algorithm will be introduce to speed-up the calculation and convergence.

Haizhao Yang
Duke University
Math Dept, Duke University
haizhao@math.duke.edu

MS35
Optimization on Flag Manifolds

Flag manifolds are generalization of Grassmannian manifolds. In this talk, I will discuss a framework of optimization on flag manifolds. The idea is to apply results in Riemannian geometry about homogeneous spaces to flag manifolds so that we can do optimization such as deepest descent or gradient descent on flag manifolds explicitly. This talk is based on a joint work with Lek-Heng Lim and Ken Sze-Wai Wong.

Ke Ye
Chicago University
kye@galton.uchicago.edu

Lek-Heng Lim, Ken Sze-Wai Wong
University of Chicago
lekheng@galton.uchicago.edu, kenwong@uchicago.edu

MS36
How to Validate Your Molecular Model (and Why You Should Do It!)

Validation and verification are companion processes in assuring the quality and reproducibility of numerical simulations. While verification tends to focus on software, validation is intended to ensure that the model we are simulating accurately reflects the behaviors of the system we are studying. Failure to validate numerical modeling can have catastrophic consequences, as exhibited by the 1998 Mars Climate Orbiter mission, as well as other engineering failures. We discuss the basic principles underlying the validation process, and present examples from our research groups on how the validation process can be applied to molecular simulations.

Ahmed E. Ismail
Department of Chemical and Biomedical Engineering
West Virginia University
ahmed.ismail@mail.wvu.edu

Christoph Klein
Department of Chemical and Biomolecular Engineering
Vanderbilt Universtity
christoph.klein@vanderbilt.edu

Janos Sallai
Institute for Software Integrated Systems
Vanderbilt University
janos.sallai@vanderbilt.edu

Christopher Iacovella
Vanderbilt University
christopher.r.iacovella@vanderbilt.edu

MS36
Molecular Simulation and Correlation of Thermodynamic Data

Molecular simulation attempts to predict thermophysical

properties from scratch. The only input are molecular models and their interactions. One desire is to reduce experimental efforts (years) by orders of magnitude (days). The present work demonstrates that any thermodynamic property can be rigorously and simultaneously measured in any proper statistical mechanical ensemble. The methodology is based on the measurement of the non-redundant set of fundamental equation of state derivatives, such as derivatives of entropy or Helmholtz energy with respect to energy, volume, and temperature. Those derivatives are fundamental ensemble averages, resulting in essentially complete thermodynamic information, exhausting statistical mechanical possibilities. In the canonical ensemble the methodology results in ultimate efficiency for fundamental equation of state correlation. Existing molecular simulation codes can be augmented by the methodology as modules. The presentation outlines the fundamentals of the methodology and gives numerical examples. Strategies to correlate small or large thermodynamic data sets are discussed.

Rolf Lustig
Cleveland State University
Chemical and Biomedical Engineering
r.lustig@csuohio.edu

MS36

The NIST Standard Reference Simulation Website: Reference Calculations and Evaluated Thermodynamic Properties to Aid Molecular Simulation Users

Monte Carlo and molecular dynamics simulation are methods for computing the properties of some kind of system, for which the intermolecular interactions are specified, via mathematical relationships derived from statistical mechanics. Since statistical mechanics itself makes no reference to molecular simulation of any kind, the properties should not depend on the simulation algorithm used for a specified model. Consequently, the results obtained from a molecular simulation should be characteristic of the of the model system, subject only to statistical uncertainty, provided that the simulation technique follows the necessary rules and is computationally robust. Standardized results for molecular simulations are, then, achievable. Yet, there are few examples of standard molecular simulation results available to users. In this work, we discuss efforts at NIST to produce the "NIST Standard Reference Simulation Website" [Shen, V.K., Siderius, D.W., and Krekelberg, W.P., eds., NIST Standard Reference Simulation Website, http://www.nist.gov/mml/csd/informatics_research/srsw.cfm]. The goal of this ongoing project is to publish well-documented simulation results for reliable simulation software for a variety of systems that can be treated similar to "standard reference data" generated in an laboratory setting. The data provided by this NIST project may be used to validate and test molecular simulation software, as reference data, or for other applications.

Harold Hatch, William Krekelberg, Raymond Mountain, Vincent Shen
National Institute of Standards and Technology
harold.hatch@nist.gov, william.krekelberg@nist.gov, raymond.mountain@nist.gov, vincent.shen@nist.gov

Daniel Siderius
National Institute of Standards and Technology
Chemical Informatics Research Group
daniel.siderius@nist.gov

MS36

Code Users Versus Code Developers: A Fake Distinction?

In the field of atomistic simulation, we often distinguish research who work on the development of codes and algorithms from those who simply use codes written by others to solve problems. In my view, this is a false distinction because problems that can be solved by simply running a calculation using freely available codes are, by their very nature, trivial. Similarly writing software in the hope that it will be adopted by the community and without a clear application in mind is an exercise in futility. In short, this distinction fails to acknowledge that modeling any phenomenon usually requires a combination of code development and a use of code written by others. In my talk, I will, therefore, give my views on how we should write flexible and modular code that can be easily modified by others and how we should train scientists working in these fields so that they can engage with both the application side and the development side of our work.

Gareth A. Tribello
Queen's University Belfast
Atomistic Simulation Centre
g.tribello@qub.ac.uk

MS37

Polynomial Surrogates for Electrical Impedance Tomography

Electrical impedance tomography aims at reconstructing the internal conductivity of a physical body based on measurements of current and potential at a finite number of electrodes attached to its boundary. Solving the inverse problem of impedance tomography by some regularized output least squares algorithm typically requires repetitively evaluating the corresponding forward map and its derivatives with respect to the unknown parameters, which can be computationally expensive. This talk considers forming polynomial surrogates for both the forward and regularized inverse maps of impedance tomography in order to speed up the reconstruction process. The employed computational techniques include (stochastic) collocation finite element methods and adaptive tensor product quadratures.

Nuutti Hyvonen
Aalto University
Department of Mathematics and Systems Analysis
nuutti.hyvonen@aalto.fi

MS37

Directional Observability for Electrical Impedance Tomography

Under the assumption that the system is time invariant, the inverse of the finite element model of the domain, taking into account current patterns, electric potential measurements strategy and electrode placement, can be decomposed as observability times controllability matrices. The very same numerical model can be decomposed by singular value decomposition. Comparing these two decompositions, the square root of singular values can be interpreted as directional observability figures of merit. Reconstructions using data from numerical simulations illustrate the

usefulness of the figures of merit to predict image quality.

Raul G. Lima
University of São Paulo
lima.raul@gmail.com

Olavo L. Silva
University of Sao Paulo
olavo.luppi@uol.com.br

Fernando S. Moura
University of Sao Paulo
Polytechnic School - Mechanical Engineering Department
fernandosmoura@gmail.com

Erick Camargo
University of Sao Paulo
edlbcamargo@yahoo.com.br

MS37
Adapting Calderón's Method for Real-Time, Patient-Specific Imaging

Calderón's method is a linearized reconstruction method for electrical impedance tomography (EIT). Until very recently, this method has most frequently been used as a teaching tool to introduce the inverse problem in circular domains. In this talk, Calderón's method is adapted to account for patient-specific domains with a real-time image reconstruction implementation. Results from both tank and human data will be shown.

Peter A. Muller
Colorado State University
muller@math.colostate.edu

Jennifer L. Mueller
Colorado State University
Dept of Mathematics
jennifer.l.mueller@gmail.com

Michelle Mellenthin
Department of Bioengineering
University of Colorado Denver
michelle.mellenthin@ucdenver.edu

MS37
Novel Algorithms for the Development of a Combined Ultrasound and Eit Breast Imaging System

This talk discusses three novel algorithms that have been investigated for the development of a combined Ultrasound (US) and Electrical Impedance Tomography (EIT) breast imaging system. Specifically, 1) a regularization algorithm for open domains, 2) rotational EIT (rEIT), and 3) soft-prior regularization algorithms for breast imaging domains have been developed and investigated. Breast cancer is the most common cancer among American women, excluding skin cancers. The current standard method for breast cancer screening is x-ray mammography. It is a very important tool, but particularly for women with dense breasts it has higher rates of false negatives and false positives. Ultrasound (US) is a promising alternative, and the recent innovation of Automated Whole Breast (AWB)-US mitigates several issues of US while creating the opportunity for a combination with EIT. The resulting modality beyond potentially improving US would be low-cost, portable, and non-ionizing. We consider Gauss-Newton and primal dual solutions of the EIT problem assuming L2 and L1 norms, respectively. Significant improvements are demonstrated on phantom work in a breast-shaped tank for the rEIT and soft-prior algorithms whereas the open domain algorithm is evaluated on a set of bovine tissue experiments. These results are important steps in the development of this combined AWB-US/EIT system.

Ethan K. Murphy
Dartmouth University
ethan.k.murphy@dartmouth.edu

MS38
Examining the Affect of Sexual Transmission on the Dynamics of Zika Infection

The Zika virus (ZIKV) has captured worldwide attention with the ongoing epidemic in South America and its link to severe birth defects, most notably microcephaly. ZIKV is spread to humans through a combination of vector and sexual transmission, but the relative contribution of these transmission routes to the overall epidemic remains largely unknown. Furthermore, a disparity in the reported number of infections between males and females has been observed. We develop a mathematical model that describes the transmission dynamics of ZIKV to determine the processes driving the observed epidemic patterns. Our model reveals only a minor contribution of sexual transmission to the basic reproductive number, R0. This contribution is too minor to independently sustain an outbreak and suggests that vector transmission is the main driver of the ongoing epidemic. While we find a small but intrinsic disparity between male and female case counts, the differences do not account for the vastly greater number of reported cases for females, indicative of a large reporting bias. Finally, we identify conditions under which sexual transmission may play a key role in sparking an outbreak, including temperate areas where ZIKV mosquito vectors are less prevalent.

Lauren Childs
Virginia Polytechnic Institute and State University
lchilds@vt.edu

MS38
Multistage Models in HIV Infection and Treatment

HIV infection and replication involves multiple intracellular processes. Different classes of antiretroviral drugs target different stages. Some studies showed that patients receiving the integrase inhibitor raltegravir based therapy were faster to achieve undetectable viral load than other therapy and that treatment intensification with raltegravir led to a lower viral load and an increase in 2-LTR, a marker for ongoing viral replication. In this talk, using multistage models we will provide a quantitative and systematic comparison of the effect of different drug classes on HIV decay dynamics and particularly explain the viral load decline in HIV patients treated with raltegravir-based regimens. We will also evaluate the influence of raltegravir intensification on viral load and 2-LTR dynamics in HIV patients on suppressive antiretroviral therapy.

Libin Rong
Oakland University

rong2@oakland.edu

MS38

Disease Spread on Networks: Integrating Structure and Dynamics through a Generalized Inverse

A fundamental issue for understanding disease dynamics on networks is how network structure and node characteristics combine to influence disease spread. I will discuss a generalized inverse, called the absorption inverse, that arises naturally in this context. The absorption inverse is connected to transient random walks on the graph, and can be used to derive a distance metric, centrality measures, and community detection algorithms that integrate both structure and dynamics. I will describe some of these measures, together with implications for disease dynamics. This is joint work with Karly Jacobsen.

Joseph Tien
Ohio State University
jtien@math.ohio-state.edu

MS38

Title Not Available At Time Of Publication

Abstract Not Available At Time Of Publication.

Necibe Tuncer
Florida Atlantic University
ntuncer@fau.edu

MS39

Adventures in Tree-Fitting

Abstract Not Available At Time Of Publication.

Dannie Durand
Department of Biological Science, Carnegie Mellon
Biological Sciences
durand@cmu.edu

MS39

So Many Maximum Parsimony Tree Reconciliations! How Can We Find a Small Set of Representative Solutions?

Phylogenetic tree reconciliation is widely used in the fields of molecular evolution, cophylogenetics, parasitology, and biogeography for studying the evolutionary histories of pairs of entities. Reconciliation is often performed using maximum parsimony under the DTL (Duplication-Transfer-Loss) event model. Since the number of maximum parsimony reconciliations can be exponential in the sizes of the trees, an important problem is that of finding a small number of "best' representative reconciliations. In this talk, we describe several ways of defining what constitutes a set of "best' representative reconciliations and then give polynomial time approximation algorithms for these problems.

Ran Libeskind-Hadas
Computer Science
Harvey Mudd
hadas@cs.hmc.edu

MS39

Predicting Ecological Function in the Microbiome

Using Spectral Properties of Interacting Clades

Abstract Not Available At Time Of Publication.

Russell Y. Neches
UC Davis
ryneches@ucdavis.edu

MS39

Phylogenetic Inference at the Single-Cell Level

As genomic technologies have gained an ever-greater ability to profile genetic variation on the scale of single cells, phylogenetic (evolutionary tree building) methods have proven powerful tools for making sense of these data. Adaptation of phylogenetic methods to the scale of single cells has proven particularly important in understanding the evolution of cellular populations in cancers, but also has value to similar problems arising in tissue development and regeneration. This talk will consider variations on the problem of phylogenetic inference of cellular populations, with particular focus on some of the novel challenges it presents relative to species evolution. These include challenges in developing appropriate mathematical models to describe the unusual mechanisms of single-cell evolution and the specialized kinds of data that exist to study it. They also include novel algorithmic challenges in characterizing and solving for these models in the face of complex and potentially noisy data sets. These problems will be studied primarily in the context of reconstructing tumor evolution, with additional extension to special challenges in reconstructing cell lineages in healthy developing tissues.

Russell Schwartz
Biological Sciences and Computational Biology
Carnegie Mellon University
russells@andrew.cmu.edu

MS40

Checkpoint/Restart: Why You Should Delegate it to a Specialized Library

In scientific applications, checkpoint/restart used to be an optional piece of code written by the developers, sometimes using the same interfaces and parameters as other I/Os. The increase of complexity and variety of the hardware (different ant deeper hierarchy, inclusion of Non-Volatile Memory of different types in different locations, higher and different node heterogeneity), the reduction of the storage bandwidth relative to the computing and memory capacities, the intensification of system variability (load imbalance due to power management, transient performance reduction due to congestion) and the understanding that failures in large HPC systems have complex behavior makes it extremely difficult for the application developers to optimize the performance of checkpoint/restart. As other operations that are critical for performance, such as message passing and I/O libraries, there is a necessity to delegate the checkpoint/restart responsibility to a specialized library that will be optimized for the different hardware/configuration. In this talk, we present the motivations and technical developments of the VeloC library developed in the context of the Exascale Computing Project (ECP).

Franck Cappello
ANL

cappello@mcs.anl.gov

MS40

Evaluating Parallel Application Resiliency with the Software Fault Injector, PFSEFI

Application resiliency to faults is a concern as supercomputers grow to ever larger sizes while the semiconductor industry shrinks components and carefully reduces voltage to minimize power use. Users of today's supercomputers need to plan for tomorrow's systems and the parallel software fault injection tool, PFSEFI, can help by evaluating application resiliency and vulnerability. In this talk we will discuss PFSEFI and see how insights gained from using the tool can be used to quantify application vulnerability to silent data corruption and look at techniques to improve application resilience.?

Nathan A. DeBardeleben
Los Alamos National Laboratory
ndebard@lanl.gov

MS40

A Catalog of Faults, Errors, and Failures in Extreme-Scale Systems

Building a reliable supercomputer that achieves the expected performance within a given cost budget requires a full understanding of the resilience problem to provide efficient mitigation. The Catalog project develops a fault taxonomy, catalog and models that capture the observed and inferred conditions in current supercomputers and extrapolates this knowledge to future-generation systems. To date, the Catalog project has analyzed billions of node hours of system logs from supercomputers at Oak Ridge National Laboratory and Argonne National Laboratory. This talk provides an overview of our findings and lessons learned.

Christian Engelmann
Oak Ridge National Laboratory
engelmannc@ornl.gov

MS40

Toward Resilient Asynchronous Many Task Programming Model

As semiconductor technology reaches its physical limit, the performance improvement of high performance computing systems no longer follows the predictions by Moores law. One of the viable approaches to address this stagnation is to relax the reliability of computing systems, and leave the application users to manage it. To enable this idea, programming model is essential to introduce mitigations from the failure of computing systems. Today, the major programming model is MPI (Single Program Multiple Data) model, and its resilience is managed through coordinated checkpoint and restart in which the state of a program is recovered through re-execution from the checkpoint stored in secondary storage subsystems (NVRAM and disks). The scalability of this model largely depends on the balance between the throughput of storage subsystems and the frequency of system failures. These issues are better handled through asynchronous many task (AMT) programming models that allow more uncoordinated and flexible task execution and re-execution, and abstraction of computation and data which shields the users from managing low-level system and hardware features for maintaining consistency and persistency together. In this talk, we

report our ongoing activities on the resilience of high performance AMT programming model. We will discuss the resilience techniques of MPI model and the techniques for the emergent AMT model and its variants.

Keita Teranishi
Sandia National Laboratories
knteran@sandia.gov

Nicole Slattengren
Sandia National Labs
nlslatt@sandia.gov

MS41

Recent Advances on Riccati-Feedback Control of Complex Flows with Moving Interfaces

We consider the two-phase Stefan problem that models a solid and a liquid phase separated by the moving interface. In the liquid phase, the heat distribution is described by a convection-diffusion equation, for which the convection is characterized by the Navier-Stokes equations. The interface movement is coupled with the temperature through the Stefan condition, which introduces a differential algebraic structure to the system. Together with a sharp interface representation, we define a quadratic tracking-type cost functional as a target of a control input. Our goal is the feedback stabilization of an open loop optimal control for the Stefan problem. The linear-quadratic regulator problem for a linear approximation of the system around the open loop trajectory gives rise to a differential Riccati equation (DRE), which has time varying oefficients. The solution of the DRE defines the corresponding feedback gain.

Björn Baran
Max Planck Institute for Dynamics of Complex Technical Syste
baran@mpi-magdeburg.mpg.de

Peter Benner
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany
benner@mpi-magdeburg.mpg.de

Jan Heiland
Max Planck Institute, Magdeburg
heiland@mpi-magdeburg.mpg.de

Jens Saak
Max Planck Institute for Dynamics of Complex Technical Syste
saak@mpi-magdeburg.mpg.de

MS41

Structure-preserving Finite Elements for Perfect Fluids

Perfect fluids with constant density are governed by the incompressible Euler equations. These equations can be formulated as a Lagrangian system with symmetries on the group of volume-preserving diffeomorphisms. In this talk, I will show how this interpretation can be used to design finite element discretisations which share a similar structure. In particular, this leads to an energy-conserving scheme which also possesses a discrete version of Kelvin's circulation theorem [A. Natale and C. J. Cotter, A variational H(div) finite element discretisation approach for

perfect incompressible fluids, 2016, arXiv:1606.06199].

Andrea Natale
Imperial College London
a.natale14@imperial.ac.uk

Colin J. Cotter
Imperial College London
Department of Mathematics
colin.cotter@imperial.ac.uk

MS41
Hypersurface Model of the Fracture for Nonlinear Fluid Flows

In this work, we analyze the flow filtration process of slightly compressible fluids in porous media containing fractures with complex geometries. We model the coupled fracture-porous media system where the linear Darcy flow is considered in porous media and the nonlinear Forchheimer equation is used inside the fracture. The optimal length of the fracture is analyzed using diffusive capacity, a functional that measures the performance of the reservoir. Also, we devise a model to address the complexity of the fracture geometry which examines the flow inside fractures with variable thickness on a general manifold. The fracture is represented as a parametric surface on Riemannian manifold where the thickness changes in the normal direction from the barycentric surface. Using Laplace Beltrami operator, we formulate an equation that describes the flow and then further simplifications were done. Using the model, pressure profile of a nonlinear flow is analyzed and compared with the actual pressure profile obtained numerically in order to validate the model.

Pushpi J. Paranamana
Texas Tech University
pushpi.paranamana@ttu.edu

Eugenio Aulisa, Magdalena Toda, Akif Ibraguimov
Department of Mathematics and Statistics.
Texas Tech University
eugenio.aulisa@ttu.edu, magda.toda@ttu.edu, akif.ibraguimov@ttu.edu

MS41
Macro Stokes Elements on Quadrilaterals

In this project, we construct a pair of conforming and inf-sup stable finite element spaces for the two-dimensional Stokes problem yielding divergence-free velocity approximations on general convex quadrilateral partitions. The velocity and pressure spaces consist of piecewise quadratic and piecewise constant polynomials, respectively. We show that the discrete velocity and a locally post-processed pressure solution are second-order convergent.

Duygu Sap
University of Pittsburgh
dus8@pitt.edu

Michael J. Neilan
University of Pittsburgh
Department of Mathematics
neilan@pitt.edu

MS41
Numerical Analysis of a Velocity-vorticity Method for the 2D Navier-Stokes Equations

We study a velocity-vorticity scheme for the 2D incompressible Navier-Stokes equations, which is based on a formulation that couples the rotation form of the momentum equation with the vorticity equation, and a temporal discretization that stably decouples the system at each time step and allows for simultaneous solving of the vorticity equation and velocity-pressure system (thus if special care is taken in its implementation, the method can have no extra cost compared to common velocity-pressure schemes). This scheme was recently shown to be unconditionally long-time H1 stable for both velocity and vorticity, which is a property not shared by any common velocity-pressure method. Herein, we analyze the schemes convergence, and prove that it yields unconditional optimal accuracy for both velocity and vorticity, thus making it advantageous over common velocity-pressure schemes if the vorticity variable is of interest. Numerical experiments are given that illustrate the theory and demonstrate the schemes usefulness on some benchmark problems.

Camille Zerfas
Clemson University
czerfas@clemson.edu

Leo Rebholz
Clemson University
Department of Mathematical Sciences
rebholz@clemson.edu

Mine Akbas
Middle East Technical University
miakbasb@metu.edu.tr

MS41
Geometry of Synchronization in Oscillatory Networks

Networks of rhythmic systems are prevalent in nature and human societies. Understanding dynamic features, such as synchrony, of these networked systems is important in wide-ranging applications from chronobiology and neuroscience to power systems. In this work, we develop a geometric method for analyzing synchronization of a network of oscillators. In particular, we embed the state space of the networked system onto a hypertorus and show that the synchronization trajectory of the oscillators, if synchronous, is a geodesic on the hypertorus. Moreover, the method can be used to identify synchronized subnetworks, if the entire network is not synchronous, by evaluating the velocity of the trajectory, which in turn provides an estimation of the network topology. The method provides a direct data analytics tool for analyzing network synchronization structures. Simulated data based on the Kuramoto model as well as experimental data of networks of electrochemical oscillators are generated to validate and demonstrate the applicability and robustness of the developed geometric method.

Wei Zhang, Jr-Shin Li
Washington University in St. Louis
wei.zhang@wustl.edu, jsli@wustl.edu

MS42
When is it Surprising that All Gene Trees are Unique? An Application of the Generalized Birth-

day Problem

Invariants corresponding to probabilities of sequence patterns in the leaves of phylogenetic trees are a major area of research in algebraic statistics. Allman, Degnan, and Rhodes (2011) derived invariants for probabilities of gene tree topologies evolving within a species tree under the multi-species coalescent (MSC) model. Yet gene invariants arise from a mathematical object-a probability distribution-instead of from frequencies of gene tree topologies in finite datasets. So we compare gene frequencies simulated under the MSC for multiple model conditions to biological phylogenomic datasets. Salichos and Rokas (2013) recovered 1,070 topologically distinct gene trees from 23 yeast genomes, which surprised the biological community. Through our large-scale data simulation and by deriving bounds on probabilities for gene tree discord, we show that this result is not surprising under the MSC model.

Ruth E. Davidson
University of Illinois Urbana Champaign
redavid2@illinois.edu

James H. Degnan
University of New Mexico
jamdeg@unm.edu

MS42

RNA Profiling: Extracting Structural Signals from Noisy Distributions

Accurate RNA structural prediction remains challenging, despite its increasing biomedical importance. Sampling secondary structures from the Gibbs distribution yields a strong signal of high probability base pairs. However, identifying higher order substructures requires further analysis. Profiling is a novel method which identifies the most probable combinations of base pairs across the Boltzmann ensemble. As will be shown, our combinatorial approach is straightforward, stable, and clearly separates structural signal from thermodynamic noise. This new method also has important implications for RNA secondary structure prediction accuracy, conditioning, and robustness.

Emily Rogers, Christine Heitsch
School of Mathematics
Georgia Institute of Technology
erogers8@mail.gatech.edu, heitsch@math.gatech.edu

MS42

Discrete Mathematical Models in Synthetic Biology

Synthetic biology is an interdisciplinary field in which biological "machines," designed to do a variety of useful things, are built and tested in the laboratory. Mathematical modeling plays a key role in the design and testing phases, as we can model and predict the performance of the machine much faster than we can build the living implementation. Our undergraduate students have designed, built and tested a system we call Programmed Evolution, a way of forcing cells to produce the desired small molecule (e.g., a drug for treating asthma) at an optimal rate, and not evolve away from this optimal solution. We have used mathematical and computational methods, including local search algorithms, probability models and agent-based models, to predict and interpret data from the system.

Laurie Heyer

Mathematics Department
Davidson College
laheyer@davidson.edu

MS42

A Near-Optimal Control for Stochastic Gene Regulatory Networks

One of the ultimate goals of computational biology and bioinformatics is to develop control strategies to find efficient medical treatments. One step towards this goal is to develop methods for changing the state condition of a cell into a new desirable state. Using a stochastic modeling framework generalized from Boolean Networks, this talk discusses a computationally efficient method that determines sequential combinations of network perturbations (control actions), that induce the transition of a cell towards a new predefined state. The method requires a set of possible control actions as input, every element of this set represents the silencing of a gene (node) or a disruption of the interaction between two molecules (edge). An optimal control policy defined as the best intervention at each state of the system, can be obtained using theory of Markov decision processes. However, these algorithms are computationally prohibitive for models of tens of nodes. The proposed method generates a sequence of actions that approximates the optimal control policy with high probability and with a computational efficiency that does not depend on the size of the state space of the system. The methods are validated by using published models where control targets have been identified.

David Murrugarra
University of Kentucky
murrugarra@uky.edu

MS43

Applications of Quantum Annealing in Computational Finance

This presentation will discuss the application of state-of-the-art quantum annealing technology to solving a selection of high value problems encountered in computational finance. A common property of each of these problems is that they can all be expressed as general optimization problems, which, through suitable transformations, can be reduced to the quadratic unconstrained binary optimization (QUBO) form solved by a quantum annealer. The size of optimization problem (measured in terms of the number of variables) that can be solved is dependent on several factors, including the technique used to discretize the problem variables (when converting to a QUBO) and how the problem is embedded onto the Chimera Graph topology in which the qubits of the annealer are laid out. Within the framework of portfolio optimization, different techniques for variable discretization will be presented, along with their advantages and disadvantages. Four specific applications will be discussed: multi-period mean-variance portfolio optimization; (quantum) hierarchical risk parity; feature selection for credit scoring; and tax loss harvesting.

Phil Goddard
1QB Information Technologies Inc.
phil.goddard@1qbit.com

MS43

Graph Partitioning Using the D-Wave for Elec-

tronic Structure Problems

In this work, we explore graph partitioning (GP) using quantum annealing on the D-Wave 2X machine. Motivated by a recently proposed graph-based electronic structure theory applied to quantum molecular dynamics (QMD) simulations, graph partitioning is used for reducing the calculation of the density matrix into smaller subsystems rendering the calculation more computationally efficient. Unconstrained graph partitioning as community clustering based on the modularity metric can be naturally mapped into the Hamiltonian of the quantum annealer. On the other hand, when constraints are imposed for partitioning into equal parts and minimizing the number of cut edges between parts, a quadratic unconstrained binary optimization (QUBO) reformulation is required. This reformulation may employ the graph complement to fit the problem in the Chimera graph of the quantum annealer. Partitioning into 2 parts, 2^N parts recursively, and k parts concurrently are demonstrated with benchmark graphs, random graphs, and small material system density matrix based graphs. Results for graph partitioning using quantum and hybrid classical-quantum approaches are shown to equal or outperform current "state of the art" methods.

Susan Mniszewski
Los Alamos National Laboratory
smm@lanl.gov

Hayato Ushijima-Mwesigwa
Clemson University
Los Alamos National Laboratory
hushiji@g.clemson.edu

Christian Negre
Los Alamos National Laboratory
cnegre@lanl.gov

MS43

Quantum Annealing for Traffic Flow Optimization

Quantum annealing algorithms belong to the class of metaheuristic tools, applicable for solving local search problems in terms of multivariate optimization. Hardware implementing quantum annealing, such as the quantum annealing machines produced by D-Wave, has been subject to multiple analyses in research, with the aim of verifying its usefulness for solving optimization and sampling tasks. In our work, we were concerned with evaluating the D-Wave 2X by presenting a well-known and complex real-world problem: traffic flow optimization. In our work, we show that time-critical optimization tasks, such as continuous redistribution of position data for cars in dense road networks, are suitable candidates for being effectively and efficiently solved on quantum annealing systems. Furthermore, we show that we achieve linear scaling by growing the problem by three orders of magnitude. A limiting factor is given by the number of available Qbits on the chip, in the presented case 1135, as a suitable embedding of the flow problem considering not only cars causing a traffic flow minimization but also those indirectly concerned by the redistribution had to be considered, which requires a meaningful decomposition in sub-problems in the classical world.

Florian Neukart
Volkswagen
florian.neukart@vw.com

MS43

Current Opportunities for Quantum Computers: Basics, Performance, Interfaces, and Community

Quantum computers based on quantum annealing are being used for a wide array of computational methods and applications. We briefly describe current systems and recent advances. Programming a quantum annealer requires mapping the users problem to a quadratic unconstrained binary optimization (QUBO) problem, but this mapping can be challenging for arbitrary problems. We describe emerging tools that raise the level of abstraction and assist or automate mapping to QUBO form. Important capabilities include executing hardware-unconstrained QUBOs and mapping constraint-satisfaction problems and algebraic modeling languages to QUBO form. We then present a variety of examples of tasks to which users have applied D-Wave systems. These include problems from graph theory, computer vision, and signal processing. Few if any of these users had prior experience with quantum computing, and all users went from knowing almost nothing about the D-Wave system to completing their tasks in a relatively short length of time. We finish by summarizing our knowledge to date about what types of problems appear best suited for solution on such systems.

Steve P. Reinhardt
D-Wave Systems, Inc.
sreinhardt@dwavesys.com

Scott Pakin
Los Alamos National Laboratory
pakin@lanl.gov

MS44

A Gradient Flow for Microstructure

Abstract Not Available At Time Of Publication.

David Kinderlehrer
Carnegie Mellon University
davidk@andrew.cmu.edu

MS44

Equations of Motion for Grain Boundaries

Abstract Not Available At Time Of Publication.

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS44

Hidden Lorentzian Symmetry Predicts Universality Beyond Power Laws

Abstract Not Available At Time Of Publication.

Stephen J. Watson
University of Glasgow

Stephen.Watson@glasgow.ac.uk

MS45
Kinetic Equations for Utility Sharing

We consider a risk-pooling strategy whereby individuals give a utility to another member of their group to preserve the economic viability of the recipient in the context of random disasters. Using agent-based simulations and partial differential equations based on kinetic models, we determine the best policies to prioritize the requests of needy individuals and to select appropriate donors in order to keep the most individuals viable. We show that optimal policies are different for a recovery from single disaster events and for dealing with repeated disasters over a long-term.

Kirk Kayser, Dieter Armbruster
Arizona State University
School of Mathematical and Statistical Sciences
kirk.kayser@asu.edu, dieter@asu.edu

Michael Herty
RWTH Aachen University
herty@igpm.rwth-aachen.de

Christian Ringhofer
Arizona State University
ringhofer@asu.edu

MS45
A Kinetic Approach for Computation of Correlations in Many Particle Systems

Systems of many interacting particles described by coupled ODEs with random initial conditions appear in many problems of physics, biology, social science, and economics. Direct computations for such systems are prohibitively expensive due to large number of particles and randomness requiring many realizations of their initial locations. Many important phenomena in such systems may be characterized by two-point correlation function which can be found by an appropriate truncation of the BBGKY hierarchy. I will present the derivation of such a truncation and provide comparison with classical truncations such as Kirkwood Superposition Approximation. It will be also shown that key properties of two-point correlation function are preserved by the new truncation, and numerical comparison with direct simulations of the original coupled ODE system will be presented. This is a joint work with L. Berlyand (PSU), R. Creese (PSU), and P.-E. Jabin (U. of Maryland)

Mykhailo Potomkin
Department of Mathematics
Penn State University
mup20@ucs.psu.edu

MS45
Kinetic Models for Active Biosystems

We start by introducing two discrete coupled PDE/ODE models capable of exhibiting remarkable collective behavior. First, a bacterium is represented as a point dipole subject to hydrodynamic and excluded volume interactions. Simulations and analysis of the corresponding kinetic theory reveal the physical mechanisms behind the striking decrease in effective viscosity and the nontrivial correlations emerging during collective swimming. Second a model for foraging ants is introduced illustrating a transition to a collective state and local lane formation. Both are unified by the fact that a kinetic approach provides additional insight into the self-organization of these biosystems into mesoscopic groups possessing capabilities beyond that of an individual.

Shawn D. Ryan
Department of Mathematics
Cleveland State University
s.d.ryan@csuohio.edu

MS45
Estimating the Division Rate and Kernel in the Fragmentation Equation

We consider the fragmentation equation

$$\frac{\partial f}{\partial t}(t,x) = -B(x)f(t,x) + \int_{y=x}^{y=\infty} k(y,x)B(y)f(t,y)dy,$$

and address the question of estimating the fragmentation parameters - i.e. the division rate $B(x)$ and the fragmentation kernel $k(y,x)$ - from measurements of the size distribution $f(t,\cdot)$ at various times. This is a natural question for any application where the sizes of the particles are measured experimentally whereas the fragmentation rates are unknown for amyloid fibril breakage. Under the assumption of a polynomial division rate $B(x) = \alpha x^\gamma$ and a self-similar fragmentation kernel $k(y,x) = \frac{1}{y}k_0(\frac{x}{y})$, we use the asymptotic behaviour to obtain uniqueness of the triplet (α, γ, k_0) and a representation formula for k_0. To invert this formula and obtain error estimates on our nonlinear problem,one of the delicate points is to prove that the Mellin transform of the asymptotic profile never vanishes, what we do through the Wiener-Hopf representation. We also illustrate our results with numerical simulations.

Magali Tournus
Institut Mathématiques de Marseille
mtournus@math.cnrs.fr

MS46
Direct Methods for Reconstructing Impenetrable Inclusions from Electrostatic Data

In this talk, we will discuss the use of the Linear Sampling Method to reconstruct impenetrable inclusions from Electrostatic Cauchy data. We consider the case of a perfectly conducting and impedance inclusion. In either case we see that the Dirichlet to Neumann mapping can be used to reconstruct impenetrable sub-regions. We also propose a non-iterative method to reconstruct the impedance parameter from the knowledge of multiple Cauchy pairs which can be computed from Dirichlet to Neumann mapping. Some numerical reconstructions will be presented in two dimensions. This is Joint work with William Rundell

Isaac Harris
Texas A&M University
Department of Mathematics
iharris@math.tamu.edu

William Rundell
Texas A&M University, Texas
rundell@math.tamu.edu

MS46
Achieving Video Rate for Single-Pixel Cameras Us-

ing Deep Learning

The single-pixel camera uses a single detector and a high-speed spatial light modulator rather than a conventional pixelated sensor to capture images. This approach enables low cost imaging with state-of-the-art detector technologies beyond the visible spectrum. One limitation of single-pixel cameras is the inherent trade-off between image resolution and frame rate, which demands the use of compressed sensing techniques. In this work we demonstrate the application of deep learning, using deep convolutional auto-encoder networks, as an alternative to other inverse methods to recover real-time high-resolution video at 30 frames-per-second from a single-pixel camera. We find that comparable high resolution image reconstruction can be achieved at a fraction of the time of other compressed sensing methods. This work represents a significant move towards real-time applications of computational imagers, with importance to gas sensing, 3D imaging and metrology.

Catherine F. Higham
University of Glasgow
Dept of Computer Science
Catherine.Higham@glasgow.ac.uk

Roderick Murray-Smith
School of Computing Science
University of Glasgow
roderick.murray-smith@glasgow.ac.uk

Matthew P. Edgar, Miles J. Padgett
School of Physics and Astronomy
University of Glasgow
matthew.edgar@glasgow.ac.uk,
miles.padgett@glasgow.ac.uk

MS46

Computation and Modeling in Ultrasound Tomography Reconstructions

In Ultrasound Tomography (UST) transducers around the boundary of a medium measure the scattered acoustic waves arising from transmitted pulses emitted from the transducers. UST has medical applications in breast cancer detection and imaging, in which slices of the breast are imaged with the subject lying prone, and the breast suspended in a saline-filled vessel. The technique has the advantages of being non-ionizing, fast, and comfortable. In this talk, the effects on computation time and image quality of several input excitation patterns, transducer models, and computational implementation will be compared for several reconstruction algorithms for ultrasound tomography.

Jennifer L. Mueller
Colorado State University
Dept of Mathematics
jennifer.l.mueller@gmail.com

Sergio Furuie
Dept. of Telecommunications and Control
University of Sao Paulo, Brazil
sergio.furuie@leb.usp.br

Raul G. Lima
University of São Paulo
lima.raul@gmail.com

MS46

Second Order Approximation of the MRI Signal for Single Shot Parameter Assessment

Most current methods of Magnetic Resonance Imaging (MRI) reconstruction interpret raw signal values as samples of the Fourier transform of the object. Although this is computationally convenient, it neglects relaxation and offresonance evolution in phase, both of which can occur to significant extent during a typical MRI signal. A more accurate model, known as Parameter Assessment by Recovery from Signal Encoding (PARSE), takes the time evolution of the signal into consideration. This model uses three parameters that depend on tissue properties: transverse magnetization, signal decay rate, and frequency offset from resonance. Two difficulties in recovering an image using this model are the low SNR for long acquisition times in single-shot MRI, and the nonlinear dependence of the signal on the decay rate and frequency offset. In this talk, we address the latter issue by using a second order approximation of the original PARSE model. The linearized model can be solved using convex optimization augmented with well-stablished regularization techniques such as total variation. The sensitivity of the parameters to noise and computational challenges associated with this approximation will be discussed.

Rodrigo B. Platte
Arizona State University
rbp@asu.edu

MS47

Multiscale Modeling of Defects in Atomic Monolayers Undergoing Complex Bending Deformation

We present a multiscale method for defects in low-dimensional atomic and molecular systems that undergo complex bending deformations with non-zero Gaussian curvature. Our technical strategy is based on a generalization of Objective Structures (OS); OS are a large class of nanostructures with symmetry properties that are rooted in frame-indifference. OS have many attractive features, e.g., a connection to group theory, potentially a fundamental basis in the structure of materials analogous to crystals, and so on. While OS have these attractive properties that make them valuable as a tool for multiscale modeling, they do not include extended nanostructures with Gaussian curvatures. Therefore, our technical strategy introduces a generalization of OS, that we term quasi-OS (qOS). qOS have the property that they can have Gaussian curvature, but recover the attractive properties of OS in certain key limits such as vanishing Gaussian curvature. We use qOS as a means to efficiently estimate energies and forces in large portions of the naostructure away from the defect, thereby enabling multiscale calculations for large systems. We apply the multiscale method to a problem involving defects and their interaction with imposed deformations, namely, the behavior of a dislocation in a graphene sheet. We find that the reduction in bending rigidity due to a single dislocation is about 40% in the configuration that we consider.

Kaushik Dayal
Carnegie Mellon University
kaushik@cmu.edu

Amin Aghaei

Stanford University
amin1@stanford.edu

MS47

Shape-Selective Growth of Nanoscale Materials: Insights from Multi-Scale Theory and Simulation

Achieving the controlled synthesis of colloidal nanomaterials with selected shapes and sizes is an important goal for a variety of applications that can exploit their unique properties. A deep, fundamental understanding of the phenomena that promote selective growth and assembly in these syntheses will enable tight control of nanostructure morphologies in next-generation techniques. I will discuss our efforts to understand the workings of PVP, a structure-directing polymer that facilitates the formation of selective Ag nanoparticle shapes. In these studies, we use molecular dynamics (MD) simulations to understand the solution-phase binding of PVP to Ag(100) and Ag(111) surfaces and its ramifications for nanocrystal shape. We characterize the potential of mean force and the mean first-passage times for solution-phase Ag atoms to reach PVP-covered Ag facets. Using these mean first-passage times, we predict that the kinetic Wulff shapes of large Ag nanocrystals (around 100 nm) should be {100}-faceted cubes. We also use MD simulations to characterize the interfacial free energies of PVP-covered Ag facets in solution. The thermodynamic Wulff shapes that we predict are truncated octahedra with both {111} and {100} facets. These findings are consistent with experimental observations that sufficiently small Ag nanocrystals with sizes around 20 nm exhibit {111} facets and larger nanocrystals become {100}-faceted due to kinetics in the presence of PVP.

Kristen Fichthorn
Penn State University
fichthorn@psu.edu

MS47

Discrete-to-Continuum Modeling of Supported Graphene and Lattice Mismatch

Recently, a rich collection of moire patterns has been observed in graphene grown by CCVD over flat crystalline substrates. These patterns provide information about the lattice constant mismatch between graphene and the substrate, imperfections on the surface of the substrate, and strain in the graphene layer. We model the formation of these patterns and of networks of wrinkles in supported graphene. Our model is based on a rigorous discrete-to-continuum procedure that reduces an atomistic van der Waals energy to a continuum limit retaining registry effects. We also present numerical results by which we qualitatively compare predictions of our models to discrete simulations and experimental observations available in the literature.

J. Patrick Wilber
Department of Mathematics
University of Akron
jw50@uakron.edu

Malena I. Espanol
Department of Mathematics
The University of Akron
mespanol@uakron.edu

Dmitry Golovaty
The University of Akron

Department of Mathematics
dmitry@uakron.edu

MS47

Multiscale and Hybrid Approaches in 2D-Materials Growth: Kinetic Monte Carlo, Markov Chains, and Phase Field Modeling

Carbon Nano Tubes (CNT) and Graphene form a family of structures with a broad range of electronic and mechanical properties for us to choose from. However, selective growth of individual structure remains a challenge: experiments often have little selectivity over the grown structures. Therefore, deeper understanding of the growth kinetics is in great need. On an atomistic scale, DFT provides a powerful tool in understanding the thermodynamic structures of materials. However, full DFT study of kinetics, e.g. DFT-based molecular dynamics, is too expensive. A multiscale approach is therefore necessary to study the growth kinetics. In the case of CNT, the growth process is often dictated by a few key events, to which we can apply DFT; furthermore, combined with a Markov process formalism, we are able to extract long term tendencies of the growth kinetics such as termination length. To have a larger scale understanding, we combine classical potential and Monte-Carlo methods to model material growth. This method offers an atom-by-atom picture of the complex growth dynamics; moreover, it reveals the condition which results in different grain boundaries in Graphene growth. On an even larger, macroscopic scale, the probabilistic growth behavior becomes deterministic, governed by the phase field equations. We will discuss the use of the WKC version phase field model, extended onto a curved surface, to study the control of topological defects of 2D crystals via the surface topology.

Henry Yu, Ksenia Bets, Nitant Gupta, Ming Luo, Boris Yakobson
Department of Materials Science and NanoEngineering
Rice University
sy27@rice.edu,   kb13@rice.edu,   nitant.gupta@rice.edu,
mluo@rice.edu, biy@rice.edu

MS48

An Automated Measure Transport Framework for Online Non-linear Filtering and Smoothing

We use a theory of transport between probability distributions to devise algorithms for nonlinear Bayesian filtering and smoothing. In particular, we present a semi-parametric transport representation and an adaptivity technique that yield algorithms able to balance computational cost with accuracy. Our approach requires the characterization of low-dimensional transports between a tractable reference distribution–e.g., a standard Gaussian– and target distributions represented by certain modifications of the lag–1 smoothing distributions. These transports can be combined to characterize the full smoothing or posterior distribution of a sequential inference problem in a state-space model, producing a one-pass smoothing algorithm, inherently sequential and with a computational cost that is constant over time [Spantini et al., Low-dimensional coupling of probability measures: structured variational approaches to inference, 2017]. The component transports are represented using functions of a dimension twice that of the state, and are identified through the solution of unconstrained minimization problems, thanks to an intrinsically monotone parameterization. The degrees of freedom for this parametric formulation are adaptively chosen using information gathered from the first variation of the

minimization objective, which does not require additional evaluations of the target density. We showcase the capabilities of the algorithms using examples from finance and engineering.

Daniele Bigoni, Alessio Spantini, Youssef M. Marzouk
Massachusetts Institute of Technology
dabi@mit.edu, spantini@mit.edu, ymarz@mit.edu

MS48
A Conditional Gaussian Framework for Data Assimilation and Prediction of Complex Turbulent Systems

In this talk, a conditional Gaussian framework for data assimilation and prediction of complex turbulent systems is introduced. Despite the conditional Gaussianity, such systems are nevertheless highly nonlinear and are able to capture the non-Gaussian features of nature. The special structure of the filter allows closed analytical formulae for updating the posterior states and is thus computationally efficient. Three types of applications in data assimilation and prediction conditional Gaussian turbulent systems with model error are illustrated. The first example involves filtering multiscale random rotating compressible flow fields with observations from noisy Lagrangian tracers, where a barrier in gaining the information is shown as increasing the number of the tracers and effective practical strategies are developed in filtering complex flows. Second, a physics-constrained low-order nonlinear stochastic model is developed to predict two monsoon indices with strong intermittency. Efficient data assimilation and ensemble initialization algorithms for the hidden variables facilitate skillful predictions. Furthermore, an effective algorithm for estimating the probability density functions of the conditional Gaussian systems based on data assimilation is developed, which can potentially be applied to high dimension systems. Other applications, such as parameter estimation and filtering spatial extended system, will also be briefly mentioned in the talk.

Nan Chen
New York University
chennan@cims.nyu.edu

Andrew Majda
Courant Institute NYU
jonjon@cims.nyu.edu

MS48
Multilevel Ensemble Kalman Filtering for Spatially Extended Models

The ensemble Kalman filter (EnKF) is a sequential filtering method that uses an ensemble of particle paths to estimate the means and covariances required by the Kalman filter by the use of sample moments, i.e., the Monte Carlo method. EnKF is often both robust and efficient, but its performance may suffer in settings where the computational cost of accurate simulations of particles is high. The multilevel Monte Carlo method (MLMC) is an extension of the classical Monte Carlo method, which by sampling stochastic realizations on a hierarchy of resolutions may reduce the computational cost of moment approximations by orders of magnitude. In this talk I will present our recent works on combining MLMC and EnKF to construct the multilevel ensemble Kalman filter (MLEnKF) for the setting of finite and infinite dimensional state and observation spaces. Theoretical results and a numerical studies of the perfor-

mance gains of MLEnKF over EnKF will also be shown. (Joint work with Alexey Chernov, Kody J. H. Law, Fabio Nobile, and Raul Tempone.)

Håkon Hoel
EPFL
haakonah1@gmail.com

MS48
Data Assimilation Algorithm Based on Feedback Control Theory

We investigate the effectiveness of a simple finite-dimensional feedback control scheme for globally stabilizing solutions of infinite-dimensional dissipative evolution equations introduced by Azouani and Titi. This feedback control algorithm overcomes some of the major difficulties in control of multi-scale processes: It does not require the presence of separation of scales nor does it assume the existence of a finite-dimensional globally invariant inertial manifold. We present a theoretical framework for a control algorithm which allows us to give a systematic stability analysis, and present the parameter regime where stabilization or control objective is attained. In addition, the number of observables and controllers that were derived analytically and implemented in our numerical studies is consistent with the finite number of determining modes that are relevant to the underlying physical system. We verify the results computationally in the context of the Chafee-Infante reaction-diffusion equation, the Kuramoto-Sivashinsky equation, and other applied control problems, and observe that the control strategy is robust and independent of the model equation describing the dissipative system. This is joint work with Edriss S. Titi.

Evelyn Lunasin
United States Naval Accademy
lunasin@usna.edu

MS49
Optimization and Control in Free Boundary Fluid-Structure Interactions

We consider optimization and optimal control problems subject to free and moving boundary nonlinear fluid-elasticity interactions. As the coupled fluid-structure state is the solution of a system of partial differential equations that are coupled through continuity relations on velocities and normal stress tensors, defined on the free and moving interface, the investigation (existence of optimal controls, sensitivity equations, necessary optimality conditions, etc.) is heavily dependent on the geometry of the problem, and falls into moving shape analysis framework.

Lorena Bociu
NC State University
Raleigh, NC
lvbociu@ncsu.edu

MS49
Optimal Control Problems with Symmetry Breaking Cost Functions

We investigate symmetry reduction of optimal control problems for left-invariant control affine systems on Lie groups, with partial symmetry breaking cost functions. Our approach emphasizes the role of variational principles and considers a discrete-time setting as well as the standard continuous-time formulation. Specifically, we recast

the optimal control problem as a constrained variational problem with a partial symmetry breaking Lagrangian and obtain the Euler–Poincar equations from a variational principle. By applying a Legendre transformation to it, we recover the Lie–Poisson equations obtained by A. D. Borum [*IEEE Transactions on Automatic Control*, (2016)] in the same context. We also discretize the variational principle in time and obtain the discrete-time Lie–Poisson equations. We illustrate the theory with some practical examples including a motion planning problem in the presence of an obstacle.

Rohit Gupta
Institute for Mathematics and its Applications
University of Minnesota
gupta311@umn.edu

Tomoki Ohsawa
The University of Texas at Dallas
Department of Mathematical Sciences
tomoki@utdallas.edu

Leonardo J. Colombo
Department of Mathematics, University of Michighan
ljcolomb@umich.edu

Anthony M. Bloch
University of Michigan
Department of Mathematics
abloch@umich.edu

MS49
Discrete-Time Geometric Maximum Principle

We present a version of the Pontryagin Maximum Principle for discrete-time optimal control problems on manifolds including those with mixed and state constraints. In addition we provide sufficient conditions for exact penalization and sensitivity of the value function to constraint perturbations in terms of normality of extremals.

Robert Kipka
Kent State University at Stark
North Canton, OH 44720, USA
rkipka@kent.edu

Rohit Gupta
Institute for Mathematics and its Applications
University of Minnesota
gupta311@umn.edu

MS49
Qualitative Properties of the Reachable Set for Delayed Differential Inclusions

In this talk we present results involving topological properties of the solution and reachable sets for a differential inclusion problem with time delays. Properties include compactness, contractibility, connectedness, and sensitivity with respect to the initial conditions.

Norma Ortiz-Robinson
Virginia Commonwealth University
nlortiz@vcu.edu

MS50
Discussion with SIAM Members about Math Subject Classification (MSC) Codes

The Mathematics Subject Classification (MSC) is used by Mathematical Reviews and zbMATH, as well as many journals, to categorize items in the mathematical sciences literature. The classes are used by the editors and reviewers to handle both articles and books. They are part of the search engine in MathSciNet, an important tool for researchers. Having relevant classifications helps make your work discoverable and helps editors make good editorial decisions. Mathematical Reviews and zbMATH cooperate in maintaining the MSC, and update it every ten years with input from the community. The editors invite the participation of all mathematicians in the project. This minisymposium is an important opportunity for researchers in applied mathematics disciplines to have direct input in the revision planned for MSC2020. Two editors from Mathematical Reviews will describe the MSC2020 project, answer your questions, and – most importantly – solicit your input.

Edward Dunne, Dean Carlson
Mathematical Reviews
American Mathematical Society
egd@ams.org, dac@ams.org

MS51
Soft Error in Classical PCG and its Variants: Sensitivity, Numerical Detections and Possible Recovery Policies

The Conjugate Gradient (CG) method is the method of choice for the solution of large sparse symmetric positive definite linear systems. In this work, we are interested in two aspects related to transient bit-flips that might occur on data computed by the algorithm. We first study the robustness of CG when bit-flips appear in either of the two most computationally intensive kernels that are the matrix-vector product and the preconditioner application; as well as the robustness sensitivity to the bit-flip locations in time and space. Secondly, we study the robustness and reliability of various numerical criteria to detect bit-flip in CG.

Emmanuel Agullo
INRIA
emmanuel.agullo@inria.fr

Siegfried Cools
University of Antwerpen
Belgium
siegfried.cools@uantwerpen.be

Emrullah F. Yetkin
Istanbul Technical University, Informatics Institute
efatihyetkin@gmail.com

Luc Giraud
Inria
luc.giraud@inria.fr

Wim I. Vanroose
Universiteit Antwerpen
Belgium

wim.vanroose@ua.ac.be

MS51
Bosilca and Bouteiller

Abstract Not Available At Time Of Publication.

George Bosilca
University of Tennessee - Knoxville
bosilca@icl.utk.edu

MS51
The Resiliency of Multilevel Methods on Next Generation Computing Platforms: Probabilistic Model and Its Analysis

With the the advent of exascale computing expected within the next few years, the number of components in a system will continue to grow. The error rate per individual component is unlikely to improve, however, meaning that future high performance computing will be faced with faults occurring at significantly higher rates than present day installations. Therefore, the resilience properties of numerical methods will become important factors in both the choice of algorithm and in its analysis. In this talk we present a framework for the analysis of linear iterative methods in a fault-prone environment. The effects of random node failures and bit flips are taken into account through a probabilistic model involving random diagonal matrices. Using this model, we analyze the behavior of two- and multigrid methods as well as domain decomposition solvers. Both analytic convergence estimates for these methods and simulation results will be discussed.

Christian Glusa
Brown University
christian_glusa@brown.edu

Mark Ainsworth
Division of Applied Mathematics
Brown University
Mark_Ainsworth@brown.edu

MS51
Resilience for Parallel Multigrid

Parallel multigrid methods are well suited to construct fault-robust solvers. After a processor failure, lost unknowns are recomputed with recovery algorithms that use local multigrid cycles. Faults can be fully compensated when asynchronous strategies are employed. Error estimators based on stable splittings can be used to control the recovery adaptively in parallel. On petascale supercomputers, failure scenarios for problems with up to 0.6 trillion unknowns are investigated.

Ulrich J. Ruede
University of Erlangen-Nuremberg
Department of Computer Science (Simulation)
ulrich.ruede@fau.de

Markus Huber
TU Muenchen
huber@ma.tum.de

Barbara Wohlmuth
Technical University of Munich

barbara.wohlmuth@ma.tum.de

MS52
Stochastic Model of Flagellar Length Control

We analyze a model proposed by Marshall et al. for flagellar length control. It is known from experiments on the unicellular algae Chlamydomonas that (i) its two flagella reach steady-state lengths, and (ii) the flagellar lengths are correlated since, if one flagellum is severed, the remaining flagellum grows to a longer steady-state. The Marshall model features a shared limiting pool of building blocks and an inverse length-dependent growth rate, and we demonstrate why both assumptions are necessary to reproduce the observed phenomena. We show that the deterministic model equations are non-Hamiltonian and construct a Lyapunov function to prove the existence of a unique, globally asymptotically stable steady-state. We describe the domain of validity. Upon including stochastic fluctuations, we show that the model reduces to a diagonal system of Ornstein-Uhlenbeck equations for the sum and difference in flagellar lengths. We present a lower bound for the fluctuation magnitude derived under the assumption of Poisson noise. The equations generalize to organisms with $N > 2$ flagella. The combination of a shared limiting pool and a growth rate with inverse-length dependence may serve as the mechanism for length control in other cellular contexts as well.

Thomas Fai, Ariel Amir
Harvard University
tfai@seas.harvard.edu, arielamir@seas.harvard.edu

MS52
Using Computation to Understand Insect Embryogenesis

Abstract Not Available At Time Of Publication.

Jordan Hoffmann
Harvard University
jordanhoffmann@mac.com

MS52
Noisy Coupled Oscillators of the Suprachiasmatic Nucleus

The central circadian clock in mammals is located in the suprachiasmatic nucleus (SCN). This brain region has long provided inspiration for mathematicians to study noisy coupled oscillators. A genetic-biochemical negative feedback loop allows individual cells to keep track of time. However, these oscillators are noisy and must synchronize to function as an accurate clock. Additionally, the oscillator population must entrain to external light input. Slow entrainment to a shift in the light input gives rise to the phenomenon of jet lag. In this talk, I will present a model of the timekeeping processes of the SCN, which I solve using a novel numerical method based on a particle discretization of a non-local partial differential equation. This simulation gives us insight into the significant differences between population and individual entrainment to light input particularly when considering the intrinsic noise present in the system.

Adam Stinchcombe
University of Michigan

stinch@umich.edu

MS52

Glioblastoma Recurrence and Resistance to Temozolomide

Glioblastoma (GBM), the most common primary brain tumor, is extremely aggressive, killing half of all patients within a year of diagnosis and nearly all patients within two years. Typically GBM is treated with Temozolomide (TMZ), a cytotoxic drug that damages DNA and triggers cell death. We have studied the mechanisms of resistance to TMZ and used this information to model the evolution of resistance in GBM. We use two-type branching process to model the treatment and recurrence of GBM, and we have parameterized the model using experimental data. We incorporate a typical treatment plan consisting of surgery, concurrent radiotherapy, and adjuvant chemotherapy and use the model to analyze the heterogeneity within the tumor, to predict recurrence timing, and to optimize the dosing schedule with respect to recurrence time.

Kathleen Storey, Jasmine Foo, Kevin Leder
University of Minnesota
store050@umn.edu, jyfoo@umn.edu, lede0024@umn.edu

Russell Rockne
Beckman Research Institute
rrockne@coh.org

Atique Ahmed
Northwestern University
atique.ahmed@northwestern.edu

Andrea Hawkins-Daarud
Mayo Clinic Scottsdale
andjhawkins@gmail.com

MS54

Centrality Measures for Multiplex Networks Based on Eigenvectors of Multi-Homogeneous Maps

Several popular centrality measures for nodes in networks, such as the Bonacich score or the HITS centrality, are defined in terms of eigenvectors or singular vectors of matrices related to the edges in the underlying graph. In this talk we propose novel centrality measures for the nodes in multiplex networks that extend some of these well-known eigenvector centrality measures for mono-layer networks. We move from single-layer to multilayer networks by considering the positive eigenvector of suitable multi-homogeneous maps defined in terms of the adjacency tensor of the network. We prove existence and uniqueness of the centrality vectors under very mild assumptions on the topology of the edges in the multiplex graph. Extensive numerical tests are provided that compare the new ranking method to other eigenvector-like centrality measures present in the literature.

Francesca Arrigo
University of Insubria
francesca.arrigo@strath.ac.uk

Antoine Gautier
Saarland University
antoine.gautier@uni-saarland.de

Francesco Tudisco

Dept. of Mathematics
University of Padua
tudisco.francesco@gmail.com

MS54

Generative Model for Mesoscale Structure in Multilayer Networks

Multilayer networks are a way to represent diverse and interdependent connectivity patterns e.g., time-dependence, multiple types of interactions, or both that arise in many applications and which are difficult to incorporate into standard (i.e., single-layer) network representations. In the study of multilayer networks, it is common to investigate mesoscale (i.e., intermediate-scale) structures, such as dense sets of nodes connected sparsely to each other known as communities, to discover network features that are not apparent at the microscale (e.g., individual entities) or the macroscale (e.g., total edge weight). A variety of methods and algorithms are available to identify communities in multilayer networks, but they differ in their definitions and/or assumptions of what constitutes a community, and many scalable algorithms provide approximate solutions with little or no theoretical guarantee on the quality of their approximations. Consequently, it is important to develop generative models of networks to use as a common test of mesoscale-structure-detection tools. We introduce a generative model for mesoscale structure in multilayer networks that can explicitly incorporate dependency structure between layers. We discuss the parameters and properties of our generative model, and illustrate its use by comparing a variety of community-detection methods for time-dependent networks.

Marya Bazzi
Mathematical Institute
University of Oxford
maryabazzi@gmail.com

Lucas Jeub
Indiana University Bloomington
ljeub@iu.edu

Sam Howison
OCIAM, Oxford University
howison@maths.ox.ac.uk

Alex Arenas
URV, Tarragona, Spain
alexandre.arenas@urv.cat

Mason A. Porter
UCLA
mason@math.ucla.edu

MS54

Methods for Analyzing Higher-Order Structures in Networks

Random walks and spectral clustering are well-known tools to analyze network information. We will discuss a variety of generalizations of these analytical tools to higher-order structures in networks and higher-order information more generally.

David F. Gleich
Purdue University
dgleich@purdue.edu

Austin Benson
Stanford University
arbenson@stanford.edu

MS54

Detectability of Community Structure in Multi-layer and Temporal Networks Undergoing Layer Aggregation

Inspired by real-world networks consisting of layers that encode different types of connections, such as a social network at different instances in time, we study community structure in multilayer networks. We study fundamental limitations on the detectability of communities by developing random matrix theory for the dominant eigenvectors of matrices that encode random networks. Specifically, we study modularity matrices that are associated an aggregation of network layers. Layer aggregation can be beneficial when the layers are correlated, and it represents a crucial step for discretizing time-varying networks (whereby time layers are binned into time windows). We explore two methods for layer aggregation: summing the layers adjacency matrices and thresholding this summation at some value. We identify layer-aggregation strategies that minimize the detectability limit, indicating good practices (in the context of community detection) for how to aggregate layers, discretize temporal networks, and threshold pairwise-interaction data matrices.

Dane Taylor
Department of Mathematics
University of North Carolina at Chapel Hill
dane.r.taylor@gmail.com

Rajmonda Caceres
Lincoln Laboratory
Massachusetts Institute of Technology
rajmonda.caceres@ll.mit.edu

Peter J. Mucha
University of North Carolina Chapel Hill
mucha@unc.edu

MS55

Branching Polytopes for RNA Sequences

RNA is part of several intracellular processes, ranging from protein encoding to gene expression. Predicting the structure into which an RNA sequence folds would aid in understanding these processes. One of the models for secondary structure prediction relies on finding a structure which minimizes the overall free energy. In this talk we present the branching polytopes arising from considering a linearized version of a Nearest Neighbor Thermodinamic Model. We prove some structural results about these polytopes and also report on computations that were carried out on several real RNA sequences.

Fidel Barrera-Cruz, Christine Heitsch
School of Mathematics
Georgia Institute of Technology
fidelbc@math.gatech.edu, heitsch@math.gatech.edu

Svetlana Poznanovikj
Mathematical Sciences
Clemson University

spoznan@clemson.edu

MS55

The Geometry of Sloppiness

The use of mathematical models in the sciences often require the estimation of unknown parameter values from data. Sloppiness provides information about the uncertainty of this task. We develop a precise mathematical foundation for sloppiness and define rigorously its key concepts, such as 'model manifold' in relation to concepts of structural identifiability. We redefine sloppiness conceptually as a comparison between the premetric on parameter space induced by measurement noise and a reference metric on parameter space. This opens up the possibility of alternative quantification of sloppiness beyond the traditional use of the Fisher Information Matrix, which implicitly assumes infinitesimal measurement error and an Euclidean parameter space. We illustrate the various concepts involved in the proper definition of sloppiness with examples of ordinary differential equation models with time series data arising in mathematical biology.

Emilie Dufresne
University of Oxford
emilie.dufresne@nottingham.ac.uk

Heather Harrington
Mathematical Institute
University of Oxford
harrington@maths.ox.ac.uk

Dhruva Raman
University of Cambridge
dhruva.raman@eng.cam.ac.uk

MS55

Detecting Reoccurring Patterns of Scrambled Genes

DNA recombination occurs at both evolutionary and developmental levels, and is often studied through model organisms such as ciliate species *Oxytricha* and *Stylonychia*. These species undergo massive genome rearrangements during their development of a somatic macronucleus from a zygotic micronucleus. We use graphs and words to represent the rearrangement process and we investigate genome-wide the range of scrambled gene architectures that describe the precursor-product relationships. We find that there are two general patterns, reoccurring genome wide, that describe over 90% of the *Oxytricha*'s scrambled genes. We further investigate the patterns of interleaving genes and find that there are specific star-like graph structures that describe most complex interleaving patterns.

Natasha Jonoska
University of South Florida
Department of Mathematics and Statistics
jonoska@usf.edu

Masahico Saito
University of South Florida
saito@usf.edu

MS55

Recovering the Treelike Trend of Evolution Despite

Extensive Lateral Genetic Transfer

Reconstructing the tree of life from molecular sequences is a fundamental problem in computational biology. Modern data sets often contain large numbers of genes. That complicates the reconstruction because different genes can have different evolutionary histories. This is the case, in particular, in the presence of lateral genetic transfer (LGT) where a gene is inherited from a distant species rather than an immediate ancestor. Such an event produces a gene tree which is distinct from (but related to) the species phylogeny. We show that, under a natural stochastic model of LGT, the species phylogeny can be reconstructed from gene trees despite surprisingly high rates of LGT. There is however a phase transition. Once the rate of transfer crosses a threshold, the reconstruction problem requires significantly more data.

Constantinos Daskalakis
MIT
costis@csail.mit.edu

Sebastien Roch
UW Madison
Department of Mathematics
roch@math.wisc.edu

MS56
Efficient Numerical Methods for Multi-dimensional Space Fractional Semi-linear Partial Differential Equations

The fractional nonlinear Schrdinger equation (FNLSE) fractionally generalizes the classical Schrdinger equation, which is a canonical model describing various physical phenomena such as the hydrodynamics, the nonlinear optics and the BoseEinstein condensate. The FNLSE was first introduced by Laskin (2000) replacing Brownian trajectories in Feynman path integrals (corresponding to the classical Schrdinger equation) by the Lvy flights. Correspondingly, this equation includes a space fractional derivative of order a ($1 < a < 2$) instead of the Laplacian in the classical Schrdinger equation. A rigorous derivation of the space FNLSE can also be found in Kirkpatrick et al(2013). In this talk a local extrapolation of exponential operator splitting scheme is introduced to solve multi-dimensional space-fractional nonlinear Schrodinger equations. The reliability and adaptability of the proposed methods are tested by implementing on systems of space-fractional nonlinear Schrodinger equations including space-fractional Gross-Pitaevskii equation, which is used to model optical solitons in graded-index fibers. Numerical experiments are shown to demonstrate the efficiency, accuracy and reliability of the method on large scale systems.

Abdul Qayyum M. Khaliq
Middle Tennessee Sate University
Abdul.Khaliq@mtsu.edu

MS56
An Exploration of Quenching-Combustion Via Globalized Fractional Models

Singular reaction-diffusion partial differential equations have played an important role in the modeling of solid-fuel combustion processes, electric current transients in polarized ionic chambers, and enzyme kinematics for which singularities develop as the solution evolves in time. It has been recently noted that these type of physical phenomena may be approximated more accurately if naturally balanced fractional derivatives are used. This talk will focus on the resulting fractional quenching-combustion equations. Novel numerical results will be presented. Preliminary analysis concerning certain key features when second-order fractional derivative operators oriented from both left-sided and right-sided α-th order formulations, $0 \leq \alpha \leq 2$, will be given.

Joshua Padgett
Baylor University, USA
josh_padgett@baylor.edu

Qin Sheng
Department of Mathematics
Baylor University
Qin_Sheng@baylor.edu

MS56
An Efficient Probabilistic Numerical Method Based on Fourier-Cosine Series for Fractional Laplacian Equations

We develop a probabilistic numerical scheme based on Fourier-cosine series to solve linear and semi-linear fractional Laplacian equations in unbounded domains. Since the fractional Laplacian operator is the infinitesimal generator of the standard symmetric alpha stable process, the temporal discretization leads to an induction time-stepping scheme involving conditional expectations with respect to the alpha stable process. Those expectations are approximated using the Fourier cosine series expansions, relying on the availability of the characteristic function of the stochastic process. We provide error estimates of the numerical error of our scheme in the one-dimensional case. The proposed method is applied to solve one- and two-dimensional fractional Laplacian equations in unbounded domains, in order to demonstrate its effectiveness and efficiency.

Guannan Zhang
Oak Ridge National Laboratory
zhangg@ornl.gov

MS57
GPU-Accelerated Stochastic Models of Cardiac Myocytes to Understand Genetically-Based Arrhthmia

Cardiac Arrhythmia is a major health problem worldwide that can lead to death. While deterministic modeling has given significant insight into the mechanism of some arrhythmia, there are certain components of cardiac excitation and contraction that stochastic in nature. Stochastic simulations pose large computational challenges that in the past have made such simulations impractical. We have developed our "Ultrafast Monte Carlo Algorithm" that when ported to GPU offers increases in computational efficiency that makes such calculations feasible. We have used our stochastic models of the cardiac myocytes to understand how genetic defects in a protein can give rise to an arrhythmia.

Mohsin S. Jafri
George Mason University
sjafri@gmu.edu

MS57
Near Real-Time Interactive Cardiac Simulations in

Tissue Using WebGL

Data collected from numerous countries indicate that cardiac disease is the leading cause of death not only in United States, but also globally. Simulation of the electrophysiology of the cardiac tissue involves solving a couple to a hundred stiff ODEs for each point in space depending on the complexity of the models used. The stiffness of the ODEs together with the spatial resolution constraints impose huge computational costs which can only be overcome by high performance solutions. In this talk, we show how WebGL can be used to utilize the computational power of the graphic card and transform our personal computers and even cell-phones to supercomputers to solve cardiac problems in real-time and interactively. We will demonstrate, live and in real-time, how arrhythmias can form in tissue and how can they result in fibrillation. Using this approach, we will show how simulation tools for research, diagnosis, and even education can be made instantly available to a broad audience throughout the world.

Abouzar Kaboudian, Flavio H. Fenton
Georgia Institute of Technology
abouzar.kaboudian@physics.gatech.edu,
flavio.fenton@physics.gatech.edu

MS57

CindyGL: Automatic Translation of a High-level Programming Language to a GPU Shader Language − Theory and Application

We present how a high-level programming language can be automatically translated to a shader language of the GPU. Moreover, the software CindyGL will be introduced as a working proof of concept. The challenges of automatic transcompilation include the detection of high-level code parts which are suitable for massive parallelization. In the case of an untyped high-level programming language, the transcompilation demands the determination of the types or the corresponding data structures on the GPU. Furthermore, read and write access to textures have to be detected and modeled corresponding to the hardware architecture. In our approach, the detection of the relevant code is done through recursive analysis of the syntax tree, while the types are determined by a fixed point algorithm. A sample implementation of this has been done through CindyGL, a software to author GPU-based interactive content. It is part of CindyJS, which is a framework for creating interactive (mathematical) content for the web. The core component of CindyGL is a transcompiler, which can translate the CindyJS inherent scripting language CindyScript to the OpenGL Shading Language (GLSL). With this, CindyGL leverages WebGL for parallelized computations. Among other tasks, CindyGL is used for real-time colorplots and feedback loops. With this tool, the access to various applications on the GPU, like numerical simulations of cellular automatons, raytracing and fractal generation, is made easier.

Aaron Montag, Jürgen Richter-Gebert
Chair for Geometry and Visualization (M10)
Technical University of Munich
montag@ma.tum.de, richter@ma.tum.de

MS57

Studying the Instabilities of Spiral Waves Due to Their Chirality in Anisotropic Cardiac Tissue using

CUDA

The heart is a complex system, from its geometrical shape to its electrophysiology, which present various challenges from the modeling and computational perspective. Due to its crucial role in keeping humans alive, understanding this vital organ is of utmost interest to biophysicists and quantitative biologists. In particular, we are interested in studying the stability of spiral waves in 3-dimensional anisotropic cardiac tissue. Spiral waves are known to cause arrhythmias such as tachycardia, and their breakup can lead to fibrillation which, if not treated immediately, is fatal. In this talk, we will show how CUDA can be used to program GPUs to analyze the sensibility of the waves to their chirality and how their evolution can be affected by it. Further novelty of this study is that we show how it is possible to solve implicit algorithms in the parallel realm of the GPUs to speed up integration times and achieve close to real-time simulations.

Hector Augusto Velasco Perez, Abouzar Kaboudian,
Flavio H. Fenton
Georgia Institute of Technology
hectorvelasco@gatech.edu,
abouzar.kaboudian@physics.gatech.edu,
flavio.fenton@physics.gatech.edu

MS58

Blocking Optimization Strategies for Sparse Tensor Computation

Abstract Not Available At Time Of Publication.

Jee Choi
IBM TJ Watson
jwchoi@us.ibm.com

MS58

Tensor Analysis: Applications and Algorithms

Tensor Analysis: Applications and Algorithms Abstract: Can tensors help us understand fMRI brainscans? How about computer network intrusion detection? We focus on the multiple applications that tensors can help us analyze, including co-evolving time sequences, power-grid measurements, and more. We also give a recent algorithm for higher order tensors (4 or higher), that achieves several orders of magnitude savings in space and time, and the 'groupNteach' algorithm, connecting education to matrix algebra and information theory.

Christos Faloutsos
Carnegie Mellon University
christos@cs.cmu.edu

MS58

Portability and Scalability of Sparse Tensor Decompositions on CPU/MIC/GPU Architectures

Tensors have found utility in a wide range of applications, such as chemometrics, network traffic analysis, neuroscience, and signal processing. Many of these applications have increasingly large amounts of data to process and require high-performance methods to provide a reasonable turnaround time for analysts. In this work, we consider decomposition of sparse count data using CANDECOMP-PARAFAC alternating Poisson regression (CP-APR) with both multiplicative update and quasi-Newton methods. For these methods to remain effective on modern large

core count CPU, Many Integrated Core (MIC), and Graphics Processing Unit (GPU) architectures, it is essential to expose thread- and vector-level parallelism and take into account the memory hierarchy and access patterns for each device to obtain the best possible performance. In this presentation, we will discuss the optimization and observed performance of the methods on modern high-performance computing architectures using the Kokkos programming model, overhead incurred by portability, and implications for upcoming distributed solver development.

Christopher J. Forster, Keita Teranishi, Greg Mackey
Sandia National Laboratories
cjforst@sandia.gov, knteran@sandia.gov,
gemacke@sandia.gov

Daniel M. Dunlavy
Sandia National Laboratories
Computer Science and Informatics
dmdunla@sandia.gov

Tamara G. Kolda
Sandia National Laboratories
tgkolda@sandia.gov

MS58

Model-Driven Sparse CP Decomposition for Higher-Order Tensors

Given an input tensor, its CANDECOMP/PARAFAC decomposition (or CPD) is a low-rank representation. CPDs are of particular interest in data analysis and mining, especially when the data tensor is sparse and of higher order (dimension). This paper focuses on the central bottleneck of a CPD algorithm, which is evaluating a sequence of matricized tensor times Khatri-Rao products (MTTKRPs). To speed up the MTTKRP sequence, we propose a novel, adaptive tensor memoization algorithm, AdaTM. Besides removing redundant computations within the MTTKRP sequence, which potentially reduces its overall asymptotic complexity, our technique also allows a user to make a space-time tradeoff by automatically tuning algorithmic and machine parameters using a model-driven framework. Our method improves as the tensor order grows, making its performance more scalable for higher-order data problems. We show speedups of up to 8 and 820 on real sparse data tensors with orders as high as 85 over the SPLATT package and Tensor Toolbox library respectively; and on a full CPD algorithm (CP-ALS), AdaTM can be up to 8 faster than state-of-the-art method implemented in SPLATT.

Jiajia Li
College of Computing
Georgia Institute of Technology
jiajiali@gatech.edu

Jee Choi
IBM TJ Watson
jwchoi@us.ibm.com

Ioakeim Perros
Georgia Institute of Technology
perros@gatech.edu

Jimeng Sun
College of Computing
Georgia Institute of Technology
jsun@cc.gatech.edu

Richard Vuduc
Georgia Institute of Technology
richie@cc.gatech. edu

MS59

Uncertainty Quantification and Discrepancy for Complex Multiscale Systems

Uncertainty quantification (UQ), and especially Bayesian calibration, help obtain reliable predictions for multi-scale problems. These models often must be constrained to experimental bench-scale data. The calibration framework requires discrepancy term between the model and reality, and often a stochastic emulator trained to limited output from a computationally expensive model. Here we present advancements in statistical methodology in UQ; in particular, the discussion will be about dealing with model discrepancy in small scale models or submodels and upscaling uncertainty or calibration at the large scale system level. Other possible challenges include accounting for due functional inputs and outputs, an intrusive dynamic discrepancy approach, upscaling of uncertainty for a multi scale system, and calibration problems with a large number of potential parameters. We used flexible and computationally approaches for the emulator and/or discrepancy, including a Bayesian Smoothing Spline (BSS) ANOVA Gaussian Process. The methodology presented may have far-reaching impact in many areas of science where multiscale modeling is used. This work will include applications to carbon capture systems.

K. Sham Bhat
Los Alamos National Laboratory
bhat9999@lanl.gov

David S. Mebane
Department of Mechanical and Aerospace Engineering
West Virginia University
david.mebane@mail.wvu.edu

Troy Holland, Peter W. Marcy
Los Alamos National Laboratory
tholland@lanl.gov, pmarcy@lanl.gov

Priyadarshi Mahapatra
National Energy Technology Laboratory
priyadarshi.mahapatra@netl.doe.gov

Curtis Storlie
Mayo Clinic
storlie.curt@mayo.edu

MS59

Towards Accounting for Model Error in CO2 Retrievals from the OCO-2 Satellite

The Orbiting Carbon Observatory 2 (OCO-2) collects space-based measurements of atmospheric CO_2. The CO_2 measurements are indirect, the instrument observes radiances (reflected sunlight) over a range of wavelengths and a physical model is inverted to estimate the atmospheric CO_2. This inference is in fact an estimation of physical parameters, which can be both biased and over-confident when model error is present but not accounted for. The OCO-2 mission addresses this problem in a few different ways, e.g. with a post-inference bias correction procedure based on ground measurements. This talk will discuss methods to account for informative model error directly

in the inversion procedure to lessen bias and provide more reliable uncertainty estimates.

Jenny Brynjarsdottir
Case Western Reserve University
Dept. of Mathematics, Applied Mathematics and Statistics
jxb628@case.edu

Jonathan Hobbs, Amy Braverman
Jet Propulsion Laboratory
California Institute of Technology
jonathan.m.hobbs@jpl.nasa.gov,
Amy.Braverman@jpl.nasa.gov

MS59

A Non-Intrusive Embedding Approach for Statistical Characterization of Model Error

Applications of Bayesian model calibration often assume the data are consistently generated from the model–that is, the model is correct. In reality, all models are approximations to the truth. It is thus crucial to quantify and propagate uncertainty due to the error in the model, resulting from its associated structural assumptions. Taking an engineering perspective where we focus on the model *predictions*, we introduce a model-error strategy that embeds a stochastic model error representation in select model parameters. Armed with data from higher fidelity sources, we then estimate the parameters and discrepancy simultaneously. The embedded approach is particularly advantageous for situations where predictive quantities are the focus: it generates physically meaningful predictions of quantities of interest (QoIs) that automatically respect the governing equations and physical constraints in the model, and provides an intuitive platform for "extrapolating' the model error for predicting new QoIs. Furthermore, the procedure is non-intrusive, and treats the model as a black box. Using a Bayesian perspective, the calibration problem is solved by combining techniques of approximate likelihood, adaptive Markov chain Monte Carlo, and polynomial chaos expansions. We demonstrate our method in large eddy simulations (LES) of flows inside a scramjet engine, where we study static versus dynamic Smagorinsky LES subgrid models, and 3D versus 2D geometries.

Xun Huan, Khachik Sargsyan
Sandia National Laboratories
xhuan@sandia.gov, ksargsy@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

MS59

Approximate Bayesian Inference for Intractable Likelihood Functions Due to Modeling Errors

Modeling and quantifying structural uncertainty is one of the most important and challenging issues in uncertainty quantitation. General formulations that exploit the structure of physics-based models by using internal discrepancies to capture structural errors yield intractable likelihood functions. As a result, solving the Bayesian inverse problem require MCMC in high-dimensions or nested sampling. A novel approximate sampling approach is proposed to solve the inference problem in the presence of model errors. Numerical results are provided to show also the impact of

using the proposed sampling algorithm when modeling the structural errors is completely ignored.

Xiao Lin
University of South Carolina
University of South Carolina
lin65@email.sc.edu

Gabriel Terejanu
University of South Carolina
terejanu@cse.sc.edu

MS60

High-throughput Identification and Characterization of Two-dimensional Materials using Density Functional Theory

In this work, we introduce a simple criterion to identify two-dimensional (2D) materials based on the comparison between experimental lattice constants and lattice constants mainly obtained from Materials-Project (MP) density functional theory (DFT) calculation repository. Specifically, if the relative difference between the two lattice constants for a specific material is more than 5%, we predict them to be good candidates for 2D materials. We have predicted at least 521 such 2D materials. For all the systems satisfying our criteria, we manually create a single layer system and calculate their energetics, structural, electronic, and elastic properties for both the bulk and the single layer cases. To validate our criterion, we calculated the exfoliation energy of the suggested layered materials, and we found that in 88.9% of the cases the currently accepted criterion for exfoliation was satisfied. We also performed X-ray diffraction and Raman scattering experiments to benchmark our calculation data for molybdenum telluride as a test case. At present, we have 427 bulk and 252 single layer materials in our database but many more calculations are currently underway. The data is publicly available at the website http://www.ctcms.nist.gov/ knc6/JVASP.html .

Kamal Choudhary
NIST
kamal.choudhary@nist

MS60

Steric Hindrance of Crystal Growth: Nonlinear Mesoscale Model in 1+1 Dimensions

By linking atomistic and mesoscopic scales via a stochastic approach, I will discuss how a local steric effect can hinder crystal growth on a (1+1)-dimensional surface. Starting from a many-atom master equation of a kinetic restricted solid-on-solid model, I will show how one can extract a coarse-grained, nonlinear mesoscale description that defines the motion of a line defect on the surface. This is joint work with J. Schneider and P. Patrone.

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

MS60

The Role of Topology in Microstructure-property Relationships: A 2D DEM Based Study

The problem of microstructure-property relationship (design of microstructures suitable for a given application) is

a longstanding problem in materials research. Although many contributions have been made in the past decades, several fundamental questions have only recently started gaining attention, such as how to describe the topology of microstructures, how to quantify its variability for given design conditions and how the network geometry and texture influence the material elastic/plastic response. In this work, we compare several entropy-based mesoscale approaches for characterizing 2D polycrystalline materials topology, based on the grain areas and number of sides. Then, we perform simulations of uniaxial compression loading tests on an idealized material by using a grain-level micro mechanical discrete element method (DEM) model to reveal dependence of materials elastic properties on the mesoscale topological information.

Katerine Saleme Ruiz
Department of Mathematical Sciences
George Mason University
kis14@msstate.edu

Maria Emelianenko
George Mason University
memelian@gmu.edu

MS60
Surface Elasticity in Steigmann-Ogden Form in Modeling of Fracture

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.

Anna Zemlyanova
Department of Mathematics
Kansas State University
azem@ksu.edu

MS61
Clawpack: Building An Open Source Ecosystem for Solving Hyperbolic PDEs

Clawpack is a software package designed to solve nonlinear hyperbolic partial differential equations using high-resolution finite volume methods based on Riemann solvers and limiters. The package itself has been under development for 20 years and now contains a number of variants aimed at different applications and diverse set of user communities. More recently Clawpack development has been moved to a model based on GitHub to help encourage a wider community engagement. This involvement has informed a number of design decisions leading to a more ex-

tensible and capable code base. These experiences will be discussed along with some ideas on how to apply them to other projects with similar goals.

David I. Ketcheson
King Abdullah University of Science & Technology (KAUST)
david.ketcheson@kaust.edu.sa

Kyle T. Mandli
Columbia University
Applied Physics and Applied Mathematics
kyle.mandli@columbia.edu

MS61
Experiences with Library Interoperability in the xSDK

The vision of the xSDK (Extreme-scale Scientific Software development Kit) is to provide a collection of software elements that provide the building blocks for efficient development of high-quality applications. The first release of the xSDK included four major open-source numerical libraries (hypre, SuperLU, PETSc, and Trilinos). Our goal is to enable compatibility among independently developed packages and provide interoperability by creating interfaces between the xSDK libraries. In this talk, we present the experience of the IDEAS software productivity team in creating and extending the xSDK. Topics include the various difficulties we faced, including third-party library version conflicts, circular dependencies, and how to maintain interoperability between libraries that are still under active development. We will also discuss the impact of the xSDK on scientific application developers.

Alicia M. Klinvex
Sandia National Laboratories
amklinv@sandia.gov

MS61
deal.II: Perspectives from a Modular and Community-Driven Finite-Element Library

deal.II is a C++ open-source software library supporting the creation of finite-element codes. With a development history of almost 20 years the project has nowadays a core team of 12 developers, and has seen (often regular) contributions by over 200 people over the years. Over 150 scientific publications per year utilize deal.II. This talk gives an overview of deal.II's design philosophy, developer and user community and development process. In particular, the scope of the library, its modular design and utilization of C++ features are discussed, and how these directly influence the development process and user participation. We describe resources we make available to the community that range from an extensive documentation of library routines and fully functional example programs to online discussion groups. Further, we discuss how open-source centered online services like github can be used for a peer-reviewed commit model that ensures quality and encourages user contributions.

Matthias Maier
University of Minnesota Twin Cities
msmaier@umn.edu

MS61
Numerical Libraries: Community Achievements,

Challenges, and Opportunities

Numerical libraries have proven effective in providing widely reusable software that is robust, efficient, and scalable—delivering advanced algorithms and data structures that enable scientific discovery for a broad range of applications. As we collectively address more advanced modeling, simulation, and analysis, the developers of open-source numerical libraries are increasingly encouraging community contributions to their software, and at the same time considering more effective strategies for connections with external packages that provide complementary functionality. The speakers in this session will discuss strategies for numerical library design and development that promote extensibility and community contributions. We will also discuss challenges and opportunities in working toward broader community scientific software ecosystems.

Lois Curfman McInnes
Mathematics and Computer Science Division
Argonne National Laboratory
curfman@mcs.anl.gov

Michael Heroux
Sandia National Laboratories
maherou@sandia.gov

MS62

Implicit Bias Its Impact on the Proposal Review Process: The View from NSF

Abstract Not Available At Time Of Publication.

Ron Buckmire
Division of Undergraduate Education
National Science Foundation
rbuckmir@nsf.gov

MS62

Gender Issues and the Impact of Implicit Bias in Appointments, Promotions, Peer Review and Leadership Opportunities

Abstract Not Available At Time Of Publication.

Nicholas P. Jewell
Biostatistics and Statistics
University of California, Berkeley
jewell@berkeley.edu

MS62

Stereotyping, Implicit Bias, and Experiences of Women and Underrepresented Minorities in STEM Fields

Abstract Not Available At Time Of Publication.

Denise Sekaquaptewa
Department of Psychology
University of Michigan, Ann Arbor
dsekaqua@umich.edu

MS63

A Data Assimilation Approach to Completing Models of Pattern-generating Networks

We employ a method of statistical data assimilation to estimate electrophysiological properties of neurons, the weights of their synaptic connections, and their synaptic reversal potentials in a multi-modal pattern-generating network model. We then use these estimates to predict the mode of activity that the network is currently expressing. These experiments are designed to ascertain what information regarding the network properties can, in principle, be inferred via voltage-sensitive dyeing - a technique currently in development. To that end, the measurements provided to the model are simulated time series of membrane voltage of each cell in the network. The results indicate that, with a proper construction of a transfer function associating a model state variable with an optical signal, this new imaging modality has the potential to map functional connectivity and electrophysiology in small neuronal networks.

Eve Armstrong
University of CA, San Diego
University of CA, San Diego
earmstrong@physics.ucsd.edu

MS63

Stochasticity in Vesicle Exocytosis Downstream of Ca2+ Channel Gating: A Computational Study

Calcium-triggered fusion between vesicle and cell membranes, known as exocytosis, underlies synaptic neurotransmitter release, endocrine hormone release, and other critical cell mechanisms. Although this is one of the most fundamental physiological processes, with identified molecular components, its properties are still not fully understood. One distinguishing aspect of exocytosis in general and neurotransmitter release in particular is its high degree of variability. While stochastic Ca2+ channel gating is the primary source of such variability, the process is also highly variable downstream of channel gating. This variability is of great biological importance, and poses an interesting topic for mathematical investigation. It is explained by the small number of Ca2+ ions entering the cell through a single channel, co-localization between channels and vesicles, and inherent stochasticity in Ca2+ binding to Ca2+ buffers and neurotransmitter release sensors. Recently there have been several studies of stochastic properties of Ca2+ buffering, as well as computational studies of synaptic neurotransmitter release. In this talk we will summarize recent results, and present new work on the degree of variability caused by different stages in Ca2+ diffusion, buffering and sensing, and the related question of the discrepancy between trial-averaged stochastic simulations and deterministic reaction-diffusion simulations of buffered Ca2+ diffusion. Supported by NSF DMS-1517085

Victor Matveev
Dept. of Mathematical Sciences
New Jersey Institute of Technology
matveev@njit.edu

MS63

Complexity Reduction for Ion Channel Models Via Stochastic Shielding

Nerve cells produce electrical impulses ("spikes") through the coordinated opening and closing of ion channels. Markov processes with voltage-dependent transition rates capture the stochasticity of spike generation at the cost of complex, time-consuming simulations. Schmandt and Galán introduced a novel *stochastic shielding* approximation as a fast, accurate method for generating approximate sample paths with excellent first and second moment agree-

ment to exact stochastic simulations [Schmandt and Galán, Phys. Rev. Lett., 2012]. We previously analyzed the mathematical basis for the method's remarkable accuracy, and showed that the stationary variance of the occupancy at each vertex in the ion channel state graph could be written as a sum of distinct contributions from each edge in the graph [Schmidt and Thomas, J. Math. Neurosci., 2014]. The talk will present new results on the robustness of the stochastic shielding approximation, and the behavior of the related edge-importance measure, under conditions of timescale separation, population sparsity, and "bursty" ion channel behavior.

Deena Schmidt
University of Nevada, Reno
Department of Mathematics
drschmidt@unr.edu

Roberto F. Galan
Case Western Reserve University
Department of Neurosciences
rfgalan@case.edu

Peter J. Thomas
Case Western Reserve University
pjthomas@case.edu

MS63
A Benefit of Noise in Synaptic Vesicle Release

Noise is not only a source of disturbance, but it also can be beneficial for neuronal information processing. The release of neurotransmitter vesicles in synapses is an unreliable process, especially in the central nervous system. Here we show that the probabilistic nature of neurotransmitter release directly influences the functional role of a synapse, and that a small probability of release per docked vesicle helps reduce the error in the reconstruction of desired signals from the time series of vesicle release events.

Calvin Zhang
Department of Mathematics
University of Arizona
calvinz@math.arizona.edu

Charles S. Peskin
Courant Institute of Mathematical Sciences, New York Univers
peskin@cims.nyu.edu

MS65
Bayesian Uncertainty Quantification in the Classification of High Dimensional Data

Abstract Not Available At Time Of Publication.

Gloria Meng
UCLA
mzhy@math.ucla.edu

Andrea L. Bertozzi
UCLA Department of Mathematics
bertozzi@math.ucla.edu

MS65
Fast Algorithms for Elastic Shape Analysis

We propose fast iterative algorithms to compute elastic shape distances between closed curves. The shape distance is based on the square-root velocity functions proposed by Srivastava et al (PAMI,2011), and is invariant to scaling, translation, and rotation. We pose the distance computation as an energy minimization problem, where we compute the optimal seed, rotation, and diffeomorphism. We develop alternating iterations, using fast dynamic programming and nonlinear optimization for the diffeomorphism, and FFT for the seed and the rotation. Our algorithm results in subquadratic running times with respect the number of nodes of the curves.

Gunay Dogan
Theiss Research, NIST
gunay.dogan@nist.gov

Javier Bernal, Charles Hagwood
National Institure of Standards and Technology
javier.bernal@nist.gov, charles.hagwood@nist.gov

MS65
A Learning Approach for Computing Regularization Parameters for General-Form Tikhonov Regularization

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

Malena I. Espanol
Department of Mathematics
The University of Akron
mespanol@uakron.edu

Julianne Chung
Department of Mathematics
Virginia Tech
jmchung@vt.edu

MS65
Density Based Clustering Applied to Image Segmentation

We discuss an approach to image segmentation based on clustering, in which we cluster a small representative sample of the data and then use classification as a way to label the remaining data points. To begin, a representative sample is identified by computing the density of the data points and using rejection sampling. We then apply persistent Continuous K-nearest neighbor (CkNN) clustering on this sample and use these as labels for the classification of the rest of the data points. We present preliminary results of this method applied to image segmentation problems.

Marilyn Vazquez
George Mason University
mvazque3@masonlive.gmu.edu

MS66
Walk This Way

Two key challenges in network science are detecting com-

munities and assigning centrality values to nodes. In both cases, the concept of a walk around the network has proved useful; through the dynamics of random walks or the combinatorics of deterministic walks. In this talk I will argue that some types of walk are less relevant than others. In particular I will restrict attention to nonbacktracking walks. This will lead to new network centrality measures. Defining, analyzing and implementing these new methods combines ideas from graph theory, matrix polynomial theory and sparse matrix computations. I will show that eliminating backtracking walks can give significantly different centrality results that offer some quantifiable advantages, as well as improving computational complexity. Further, the topic raises many interesting theoretical questions in applied matrix theory.

Desmond J. Higham
University of Strathclyde, UK
d.j.higham@strath.ac.uk

Francesca Arrigo
University of Insubria
francesca.arrigo@strath.ac.uk

Peter Grindrod
University of Oxford, UK
grindrod@maths.ox.ac.uk

Vanni Noferini
University of Essex
vnofer@essex.ac.uk

MS66

Detecting Changes in Node Importance in Time-Evolving Networks

One of the most fundamental questions in network analysis concerns ranking the importance of nodes in complex networks. Many centrality measures have been developed to measure various aspects of node importance. However, the majority of these have been developed for use on static networks. In reality most real-world networks are evolving over time, whether slowly (protein-protein interaction networks) or extremely quickly (the internet). Understanding how a node's importance changes over time, especially large jumps in importance, can illuminate dynamics that would otherwise be hidden. We present a method of detecting changes in node importance relative to a fixed "seed' node in large, time-evolving networks by simulating random walks that are able to factor in temporal metadata in diverse ways. We show that sampling a sublinear number of random walks in the evolving network captures a change of specified magnitude that occurs over some duration of time with high probability. (Specifically, for an evolving network on n nodes with a history of length T, $O(\frac{T}{\tau\delta}\log n)$ random walkers will capture a change of size δ over a period of size τ with high probability). The use of random walks allows our method to be adaptable to networks which are large and noisy. It also allows for various interpretations of what level of importance change is meaningful: both δ and τ are variables in our algorithm.

Christine Klymko
Lawrence Livermore National Laboratory
klymko1@llnl.gov

Olivia Simpson
University of California, San Diego

oliviamsimpson@gmail.com

MS66

Community Detection Via Nonlinear Modularity Eigenvectors

Community identification in networks is a central problem arising in many scientific areas. The modularity function Q is an effective measure of the quality of a community, being defined as a set of nodes having high modularity. Community detection thus boils down to the combinatorial optimization problem of locating sets of nodes maximizing Q. This problem is known to be NP-hard thus posing the need of approximation techniques which are typically based on a linear relaxation of Q, induced by the spectrum of the modularity matrix M.In this work we propose a nonlinear

relaxation which is based on the spectrum of a nonlinear modularity operator $\mathcal{M}$. We show that extremal eigenvalues of $\mathcal{M}$ satisfy a tight Cheeger-type inequality providing an exact relaxation of the modularity function Q, however at a price of being more challenging to be computed than the extremal eigenvalues of the linear counterpart based on M. We propose a general optimization scheme for the computation of the extremal eigenvalues of $\mathcal{M}$, named Generalized RatioDCA, and we show monotonic ascent and convergence of the method to a critical value. Finally, we present extensive evaluations on synthetic and real-world datasets showing that our method is competitive to the state of the art.

Pedro Mercado
Dept. Math. and Computer Science
Saarland University
pedro@cs.uni-saarland.de

Francesco Tudisco
Dept. of Mathematics
University of Padua
tudisco.francesco@gmail.com

Matthias Hein
Saarland University
Dept. of Mathematics and Computer Science
hein@cs.uni-saarland.de

MS66

Locating the Vertices in a Three-Dimensional Space for Building a Large-Scale Visual Search Engine

Current academic search engines only provide a user with a list of popular papers rather than relevant but possibly not so well-known papers. Moreover, it is hard to understand the relationship between papers or the current research landscape from a list. In this talk, we present Etymo, a new graphic search engine which aims to solve these problems. The prototype is available at http://etymo.io/ Etymo works just like a web mapping service (e.g. Google Map), where a user can zoom in to see more related papers and zoom out to get an overview of the current research landscape. The Pagerank algorithm is based on the hyperlink graph of the web. We, on the contrary, build our knowledge graph from the high-dimensional encoding of the full text papers. Building a scalable graphic search engine is a challenging task. We need to locate millions of papers as nodes in a three-dimensional space such that similar papers are close to each other and papers are located in the 'correct' layers for zooming-in and out. We

will discuss our approach to the problem and show how different components of the engine work together. Machine learning based dimensionality reduction techniques are crucial for visualizing high-dimensional data. We compare and contrast different methods such as self-organizing map (SOP) and t-distributed stochastic neighbor embedding (t-SNE). We also show how we can exploit temporal network information to get more accurate results.

Weijian Zhang
School of Mathematics
The University of Manchester
weijian.zhang@manchester.ac.uk

Jonathan Deakin
The University of Manchester
jonathan.deakin@postgrad.manchester.ac.uk

Nicholas J. Higham
School of Mathematics
The University of Manchester
nick.higham@manchester.ac.uk

MS67

How to Improve Your Denoising Result Without Changing Your Denoising Algorithm

In this talk we will review some recent approaches for improving denoising results, in the particular case of photographic images: -We propose two different geometric frameworks, in which the original noisy image is transformed into a set of images that are easier to denoise (using local or patch-based methods), and then are transformed back into a regular, but now noise-reduced, image. -We show that a simple, local TV-based denoising method applied to a RAW image can achieve better results than patch-based methods like BM3D applied to the camera output. -We show that a simple, local denoising method based on curvature smoothing can visually outperform non-local methods on photographs with actual noise.

Marcelo Bertalmío
Universitat Pompeu Fabra
marcelo.bertalmio@upf.edu

Thomas Batard
Department of Information and Communications
Technologies
University Pompeu Fabra
thomas.batard@upf.edu

Gabriela Ghimpeteanu
Universitat Pompeu Fabra
gabriela.ghimpeteanu@upf.edu

Stacey E. Levine
duquesne university
department of mathematics and computer science
sel@mathcs.duq.edu

MS67

Learning with Privileged Information and Its Application in Medical Informatics

Vapnik et al. created a new learning paradigm in which the learner is provided with not only a set of training examples, but also additional privileged information. The privileged information in the training phase can help tune-up and improve the choice of the classification function. This type of information is abundant in healthcare, where much more information about a patients health status is available in retrospective databases compared to real-time environments.

Kayvan Najarian
Department of Computational Medicine and
Bioinformatics
University of Michigan
kayvan@med.umich.edu

Harm Derksen
University of Michigan
Department of Mathematics
hderksen@umich.edu

MS67

NIR-VIS Face Recognition Via Cross-spectral Hallucination and Low-Rank Embedding

Most face datasets accessible for training and verification are only collected in the VIS (visible light) spectrum. It remains a challenging problem to match NIR to VIS face images due to the different light spectrum. Recently, breakthroughs have been made for VIS face recognition by applying deep learning on a huge amount of labeled VIS face samples. The same deep learning approach cannot be simply applied to NIR face recognition for two main reasons: First, much limited NIR face images are available for training compared to the VIS spectrum. Second, face galleries to be matched are mostly available only in the VIS spectrum. In this paper, we propose an approach to extend the deep learning breakthrough for VIS face recognition to the NIR spectrum, without retraining the underlying deep models that see only VIS faces. Our approach consists of two core components, cross-spectral hallucination and low-rank embedding, to optimize respectively input and output of a VIS deep model for cross-spectral face recognition. Cross-spectral hallucination produces VIS faces from NIR images through a deep learning approach. Low-rank embedding restores a low-rank structure for faces deep features across both NIR and VIS spectrum. It is often equally effective to perform hallucination to input NIR images or low-rank embedding to output deep features for a VIS deep model for cross-spectral recognition. If hallucination and low-rank embedding are deployed together, state-of-the-art is obtained.

Jose Lezama, Qiang Qiu, Guillermo Sapiro
Duke University
jlezama@gmail.com, qiuqiang@gmail.com,
guillermo.sapiro@duke.edu

MS67

The Little Engine That Could: Regularization by Denoising (RED)

In this talk we present a framework that leverages existing state-of-the-art image denoising algorithms to treat other tasks in image processing, called Regularization by Denoising (RED). We propose an explicit image-adaptive Laplacian-based regularization functional, which is capable of incorporating any denoiser, treat general inverse problems, and is guaranteed to converge to the globally optimal result. The effectiveness of our approach is tested both on the image deblurring and super-resolution problems, lead-

ing to state-of-the-art results.

Yaniv Romano
EE Department, Technion
Israel
yromano@tx.technion.ac.il

Michael Elad
Computer Science Department
Technion
elad@cs.Technion.AC.IL

Peyman Milanfar
Google
peyman.milanfar@gmail.com

MS68
Parallel Graph Algorithms: Simple, Efficient and Scalable

Graph algorithms are an important tool used in a variety of applications, from DNA-sequencing to analyzing the structure and dynamics of online social networks. Unfortunately, implementing and running even the simplest graph algorithms on the massive graphs that come up in application domains is a significant challenge for users. Faced with the challenge of processing graphs at this scale, many users choose to use a distributed system to perform analysis. In this talk, we argue that graphs containing billions of vertices and hundreds of billions of edges can be simply and efficiently analyzed on commodity shared-memory servers, often with an order of magnitude improvement in runtime compared to their distributed counterparts. We present these ideas in the context of Julienne—an extension to the graph processing framework Ligra that enables us to write simple, scalable and theoretically efficient algorithms for k-core, Δ-stepping, and approximate set-cover. We show that our codes achieve up to 33x speedup over well tuned sequential baselines, and can process graphs with billions of edges in seconds and hundreds of billions of edges in minutes.

Laxman Dhulipala
Carnegie Mellon University
ldhulipa@andrew.cmu.edu

Julian Shun
University of California, Berkeley
jshun@eecs.berkeley.edu

Guy Blelloch
Computer Science Department
Carnegie Mellon University
guyb@cs.cmu.edu

MS68
Approximation Algorithms for Inventory Routing on Line Metrics

We consider the deterministic inventory routing problem over a discrete finite time horizon. Given clients on a metric, each with daily demands that must be delivered from a depot and holding costs over the planning horizon, an optimal solution selects a set of daily tours through a subset of clients to deliver all demands before they are due and minimizes the total holding and tour routing costs over the horizon. We study LP-based methods for inventory routing on line metrics. In particular, we obtain a 5-approximation

using LP rounding and a 26-approximation using primal dual. Complementing the theoretical results, we show the computational performance of our algorithms on randomly generated instances.

Yang Jiao
Carnegie Mellon University

R. Ravi
Tepper School of Business
CMU
ravi@cmu.edu

MS68
Quantum Approximation Algorithms

We outline recent and ongoing work in developing quantum approximation algorithms for graph and constraint satisfaction problems. Although Shor's quantum algorithm for integer factorization provides an exponential speedup over the best known classical algorithms, it is generally conjectured that efficient quantum algorithms are not capable of solving NP-hard problems. Thus a natural question is whether quantum algorithms may be used to provide better approximation guarantees for NP-hard discrete optimization problems than classical approximation algorithms. There are only a few quantum approximation algorithms known and none that offer better approximation guarantees over classical counterparts. Our work provides a better understanding of existing quantum approximation algorithms for problems such as maximum cut, and our broader goal is to develop quantum relaxations in the vein of convex relaxations of NP-hard problems as a basis for developing stronger quantum approximation algorithms.

Ojas Parekh
Sandia National Laboratories
odparek@sandia.gov

MS68
Cooperative Computing for Autonomous Data Centers

We present a new distributed model for graph computations motivated by limited information sharing. Two autonomous entities have collected large social graphs. They wish to compute the result of running graph algorithms on the entire set of relationships. Because the information is sensitive or economically valuable, they do not wish to simply combine the information in a single location and then run standard serial graph algorithms. We consider two models for computing the solution to graph algorithms in this setting: 1) limited-sharing: the two entities can share only a polylogarithmic size subgraph; 2) low-trust: the two entities must not reveal any information beyond the query answer, assuming they are both honest but curious. That is, they will honestly participate in the protocol, but will then learn whatever it is possible from the protocol. We present results for both models for s-t connectivity: is there a path in the combined graph connecting two given vertices s and t? In the limited-sharing model, our results exploit social network structure to exchange $O(log^2 n)$ bits, overcoming polynomial lower bounds for general graphs. In the low-trust model, our algorithm requires no cryptographic assumptions and does not even reveal node names. Time permitting, we will sketch ideas for finding dense graphs and some of the issues associated with testing on standard

test graphs.

Jonathan Berry
Sandia National Laboratories
jberry@sandia.gov

Michael Collins
Christopher Newport University
michael.collins@cnu.edu

Aaron Kearns
KBRwyle
aaron.kearns.username@gmail.com

Cynthia Phillips
Sandia National Laboratories
caphill@sandia.gov

Jared Saia
Department of Computer Science
University of New Mexico
saia@cs.unm.edu

Randy Smith
Sandia National Laboratories
ransmit@sandia.gov

MS69

A Practical Randomized CP Tensor Decomposition

The CANDECOMP/PARAFAC (CP) decomposition is a leading method for the analysis of multiway data. The standard alternating least squares algorithm for the CP decomposition (CP-ALS) involves a series of highly overdetermined linear least squares problems. We extend randomized least squares methods to tensors and show the workload of CP-ALS can be drastically reduced without a sacrifice in quality. We introduce techniques for efficiently preprocessing, sampling, and computing randomized least squares on a dense tensor of arbitrary order, as well as an efficient sampling-based technique for checking the stopping condition. We also show more generally that the Khatri-Rao product (used within the CP-ALS iteration) produces conditions favorable for direct sampling. In numerical results, we see improvements in speed, reductions in memory requirements, and robustness with respect to initialization.

Casey Battaglino
Georgia Institute of Technology
cbattaglino3@gatech.edu

MS69

Optimizing Distributed Tucker Decomposition

The Tucker decomposition generalizes the classical Singular Value Decomposition (SVD) to higher dimensional tensors. The HOSVD/HOOI methods provide a popular mechanism for computing the Tucker decomposition of a given tensor. Prior work has presented distributed implementations of these methods for both dense and sparse tensors. We shall discuss optimization strategies for both settings with the aim of reducing the computational load and the communication volume. For the dense case, our strategies are provably optimal and our experimental evaluation demonstrates that the strategies yield up to 7x performace

gain over prior implementations on practical tensors.

Venkatesan Chakaravarthy
IBM
vechakra@in.ibm.com

Jee Choi
IBM TJ Watson
jwchoi@us.ibm.com

Douglas Joseph, Xing Liu
IBM
djoseph@us.ibm.com, xliu@us.ibm.com

Prakash Murali, Yogish Sabharwal, Dheeraj Sreedhar
IBM Research - India
prakmura@in.ibm.com, ysabharwal@in.ibm.com, dhsreedh@in.ibm.com

MS69

Generalized Canonical Tensor Factorization for Binary, Count, Nonnegative, or Real-Valued Data

We consider the generalization of the canonical polyadic tensor factorization (also known as CANDECOMP, PARAFAC, or CP) to different goodness-of-fit metrics. The standard model measures fit via a squared error metric. We allow the user to generalize to other metrics that may be more appropriate for different types such as count data, binary data, or nonnegative data. This leads to a general framework for fitting the model. We show how the model can be extended to handle missing data and solved efficiently using randomized optimization methods.

Tamara G. Kolda
Sandia National Laboratories
tgkolda@sandia.gov

MS69

Decomposing Large-Scale Tensors into Rank-1 Terms Using Randomized Block Sampling

To interpret large-scale datasets, simple structures are often assumed. We focus on the decomposition of tensors into rank-1 terms, also called the (canonical) polyadic decomposition (CPD). Optimization-based algorithms used to compute the CPD are hindered by the curse of dimensionality. Many techniques based on, e.g., compression, incompleteness or parallel computation have been proposed to alleviate this curse. In this talk, we demonstrate a new strategy based on randomized block sampling. Each iteration, a random block is sampled from the tensor and a single update is computed from this block. Because of the locality property of a CPD, a block affects only few variables and updates can be computed efficiently. This process of sampling and updating is repeated up to convergence which can be determined using a novel stopping criterion based on the Cramér–Rao bound. We show how a carefully chosen step restriction schedule allows a tensor to be decomposed up to almost the same accuracy as if a state-of-the-art algorithm for a full tensor was used, while using only a fraction of the data and time compared to full tensor algorithms. The choice of this step restriction schedule can be done experimentally or using a new automated procedure. Finally, we show that, using randomized block sampling, a standard laptop suffices to decompose synthetic tensors of 8TB and real-life hazardous gas classification data within minutes while achieving high accuracy.

Nico Vervliet
Department of Electrical Engineering (ESAT)
KU Leuven
nico.vervliet@esat.kuleuven.be

Lieven De Lathauwer
KU Leuven - KULAK
lieven.delathauwer@kuleuven.be

MS70

Equivalent Inclusions in Effective Thermo-Elastic Properties of Nanocomposites Incorporating Interface Energy

In order to apply the classical micromechanics to predict the effective properties of nanocomposites incorporating interface energy, a concept of equivalent inclusion (EI) is usually adopted. The EI properties are obtained by embedding a single inclusion into an infinite matrix. However, in the existing literature there is little discussion on whether this EI is universal for different micromechanics methods. In this paper, the interface energy theory proposed by the present author is employed to investigate the applicability of the above defined EI. It is found that some elastic properties of this EI are only dependent on the properties of the inclusion and the interface, whereas others are not only dependent on the properties of the inclusion and the interface, but also on those of the matrix. The former properties of this EI can be applied to both the classical Mori-Tanaka method (MTM) and the generalized self-consistent method (GSCM). However, the latter properties can only be used in the MTM. Therefore, the above defined EI is only applicable for the MTM, and cannot be applied universally for other micromechanics methods. In this paper, a new equivalent inclusion is introduced for the GSCM and is applied to estimate the effective thermos-elastic properties of particle/fiber reinforced nanocomposites. The present results will be useful in the prediction of the effective properties of nanocomposites with interface effect by means of the micromechanics methods.

Zhuping Huang
Peking University
China
huangzp@pku.edu.cn

MS70

The Use of Layer Potentials in Solving Elasticity Problems with Surface Effects

With the development of nanotechnology the proper modelling of material surfaces becomes important. Various theoretical models have been developed to include surface effects, such as surface elasticity and surface stresses, e.g. Gurtin-Murdoch elastic model. In these models, the BVP involves standard elastic models for the bulk material supplemented by the boundary conditions in terms of jumps in displacements and/or tractions expressed via a new set of surface variables. Therefore, mathematical tools that describe the jump conditions are necessary. Such tools are readily available in the forms of elastic potentials introduced by Kupradze. For the problems under consideration, the density of a single layer potential has a physical meaning of the traction jump, while the meaning of the density of a double layer potential is that of the displacement jump. This talk describes the use of the single layer potential to the problem of an infinite elastic domain containing a circular arc with the Gurtin-Murdoch type conditions. The far field stresses are also included. The problem is reduced to a boundary integral equation, which is solved numerically by the complex variable boundary element technique using circular boundary elements.

Vladislav Mantic
University of Seville
Spain
mantic@us.es

Sofia Mogilevskaya
University of Minnesota
mogil003@umn.edu

MS70

A Chemo-Mechanics Framework for Elastic Solids with Surface Stress

Elasticity problems involving solid-state diffusion and chemo-mechanical coupling have wide applications in energy conversion and storage devices such as fuel cells and batteries. Such problems are usually difficult to solve because of their strongly nonlinear characteristics. This study first derives the governing equations for three-dimensional chemo-elasticity problems accounting for surface stresses in terms of the Helmholtz potentials of the displacement field. Then, by assuming weak coupling between the chemical and mechanical fields, a perturbation method is used and the nonlinear governing equations are reduced to a system of linear differential equations. It is observed from these equations that the mechanical equilibrium equations of the first two orders are not dependent on the chemical fields. Finally, the above chemo-mechanics framework is applied to study the stress concentration problem of a circular nano-hole in an infinitely large thick plate with prescribed mechanical and chemical loads at infinity. Explicit expressions up to the third order are obtained for the stress and solute concentration fields. It is seen from these solutions that, different from the classical elasticity result, the stress concentration factor near the nano-hole depends on the surface stress, applied tensile load and prescribed solute concentration at infinity.

Jianmin Qu
Tufts University
USA
jianmin.qu@tufts.edu

Xiang Gao
Tufts University
xiang.gao@tufts.edu

Daining Fang
Beijing University
fangdn@pku.edu.cn

MS70

Neutral Nano-Inhomogeneities in Hyperelastic Materials with a Hyperelastic Interface Model

Abstract Not Available At Time Of Publication.

Peter Schiavone
University of Alberta
Canada

pschiavo@ualberta.ca

MS71

Particle Methods for Fractional Diffusion Equations

This talk discusses the construction of deterministic particle methods for the simulation of fractional diffusion equations in unbounded domains. Various alternatives are explored, including: (a) a direct differentiation approach, (b) particle strength exchange method based on Riemann-Liouville, regularized Riesz, and Greens function representations, and (c) a diffusion velocity algorithm. Numerical simulations are used to analyze the performance of the resulting schemes and to assess their relative merits.

Samer Allouch, Marco Lucchesi
King Abdullah University of Science and Technology
samer.allouch@kaust.edu.sa, marco.lucchesi@kaust.edu.sa

Olivier Le Maitre
Laboratoire d'Informatique pour la Mécanique et les
Science
olm@limsi.fr

Kassem Mustapha
Department of Mathematics and Statistics
King Fahd University
kassem@kfupm.edu.sa

Omar Knio
King Abdullah University of Science and Technology
(KAUST)
omar.knio@kaust.edu.sa

MS71

The Finite Difference Method for Fractional Parabolic Equation with Fractional Laplacian

In this talk, we present the finite difference method for fractional parabolic equation with fractional Laplacian, where the time derivative is the Caputo derivative with derivative order in $(0, 1)$ and the spatial derivative in the fractional Laplacian. Stability, convergence, and error estimate are displayed. And the illustrative examples are provided which support the theoretical analysis.

Changpin Li
College of Sciences
Shanghai University, Shanghai, China
lcp@shu.edu.cn

MS71

Fractional-Order Models for Biological Systems With Memory

During the past three decades, the subject of fractional calculus has gained popularity and importance, mainly due to its demonstrated applications in numerous diverse and widespread fields of science and engineering. It has been successfully applied to system biology, physics, chemistry and biochemistry, hydrology, medicine and finance. This is due to the fact that modeling of such systems by fractional-order (or arbitrary-order) models provides the systems with long-time memory and gains them extra degrees of freedom. In this participation, we provide a subclass of fractional-order differential models of infectious diseases. Unconditionally, stable implicit scheme for the numerical simulations of the fractional-order delay differential model is introduced. The numerical simulations show the effectiveness of the numerical method and confirm the theoretical results

Fathalla A. Rihan
United Arab Emirates University
frihan@uaeu.ac.ae

MS71

Pricing of Options Issued on Assets Following a CGMY-Process by Solving a Forward Kolmogorov Equation

We price options when the underlying asset follows a CGMY-process. To that end, we derive the Kolmogorov forward fractional partial differential equation (FPDE) for this process. We obtain the option price by integrating the resulting probability density function multiplied by the pay-off function. Hence, we only have to solve one FPDE to price several options. This is useful in practical applications where it is common to price many options simultaneously for the same underlying process. The FPDE is discretised with a finite difference scheme in "space" and the Backward Differentiation Formula of order two in time. We will present numerical results that demonstrates the usefulness of the proposed method.

Lina von Sydow
Uppsala University
Lina.von.Sydow@it.uu.se

Josef Höök
Uppsala University, Sweden
Dept. of Information Technology
josef.hook@it.uu.se

Gustav Ludvigsson
Uppsala University
gustav.ludvigsson@it.uu.se

MS72

Learning Non-Linear Correlations Between Multi-Fidelity Models Using Deep Neural Networks

Abstract Not Available At Time Of Publication.

Ilias Bilionis
School of Mechanical Engineering,
Purdue University, West Lafayette, Indiana, 47907
ibilion@purdue.edu

Rohit Tripathy
Purdue University
rtripath@purdue.edu

MS72

Multifidelity Data Fusion As a Data-Driven Gauge Transformation

Abstract Not Available At Time Of Publication.

Ioannis Kevrekidis
Dept. of Chemical Engineering
Princeton University

yannis@princeton.edu

MS72

Multifidelity Information Fusion Via Manifold Learning

Abstract Not Available At Time Of Publication.

Seungjoon Lee
Division of Applied Mathematics, Brown University
seungjoon_lee@brown.edu

MS72

Nonlinear Information Fusion for Data-Efficient Multi-Fidelity Modeling

Abstract Not Available At Time Of Publication.

Paris Perdikaris
Massachusetts Institute of Technology
parisp@mit.edu

MS73

Uncovering Functional Relationships in Leukemia

Mass cytometers can record tens of features for millions of cells in a sample, and in particular, for leukemic cells. Many methods consider how to cluster or identify populations of phenotypically similar cells within cytometry data, but there has yet to be a connection between cell activity and other features and these groups or clusters. We use differential geometric ideas to consider how cell cycle and signaling features vary as a function of the cell populations. This consideration leads to a better understanding of the nonlinear relationships that exist in the cytometry data.

Reginald Mcgee
The Ohio State University
mcgee.278@mbi.osu.edu

MS73

A Comparison of Methods for Calculations the Basic Reproductive Number for Periodic Epidemic Systems

When using mathematics to study epidemics, often the goal is to determine when an infection can invade & persist within a population. The most common way to do so uses threshold quantities called reproductive numbers.An infections basic reproductive number (BRN), typically denoted R0, measures the infections initial ability to reproduce in a naive population, & is tied mathematically to the stability of the disease-free equilibrium.Next-generation methods have long been used to derive R0 for autonomous continuous-time systems; however many diseases exhibit seasonal behavior. Incorporating seasonality into models may improve accuracy in important ways, but the resulting nonautonomous systems are much more difficult to analyze. In the literature, two principal methods have been used to derive BRNs for periodic epidemic models. One, based on time averages is simple to apply but does not always describe the correct threshold behavior. The other, based on linear operator theory, is more general but also more complicated, & no detailed explanations of the necessary computations have yet been laid out. This paper reconciles the two methods by laying out an explicit procedure for the second & then identifying conditions (& some important classes of models) under which the two methods agree.This allows the use of the simpler method, which yields interpretable closed-form expressions, when appropriate, & illustrates in detail the simplest possible case where they disagree.

Chrsitopher Mitchell
School of Medicine
University of Utah
chris.mitchell@hsc.utah.edu

MS73

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

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

Alicia Prieto Langarica
Youngstown State University
aprietolangarica@ysu.edu

MS73

Effects of Functional Switching Within Regulatory T Cells

It is widely accepted that the primary immune system contains a sub-population of cells, known as regulatory T cells whose function is to regulate the immune response. There is conflicting biological evidence regarding the ability of regulatory cells to lose their regulatory capabilities and turn into immune promoting cells. We present a delay differential equation (DDE) model of the primary immune response to investigate the effects of regulatory T cell switching on the immune response. The model displays the usual characteristics of an immune response (expansion, contraction, and memory phases), while being robust with respect to T cell precursor frequencies. We characterize the affects of regulatory T cell switching on the peak magnitude of the immune response and identify a biologically testable range for the switching parameter. We conclude that regulatory T cell switching may play a key role in both controlling immune contraction and in the biological phenomena of immunodominance.

Shelby Wilson
Morehouse College
shelby.wilson@morehouse.edu

MS74

Future Directions for Mathematics Research within DoD

In this presentation, I will give an overview of current programs at DARPA Defense Sciences Office that have a significant focus on mathematical research and will offer some plans and thoughts as a program manager for strengthening mathematical research bases within the DoD basic research agencies.

Fariba Fahroo

DARPA, Defense Sciences Office
fariba.fahroo@darpa.mil

MS74
NSF Funding for the Mathematical Sciences: New and Changing Opportunities

The National Science Foundation supports fundamental research and education in all areas of the mathematical sciences. In addition, there are many opportunities for collaboration with other scientists and engineers. My presentation will focus on new and current programs as well as future directions in areas of interest to the SIAM community.

Deborah Lockhart
National Science Foundation
dlockhar@nsf.gov

MS74
Discussion with Audience

Abstract Not Available At Time Of Publication.

N/A N/A
N/A
N/A

MS74
DOE Long-range Planning for the Future of Applied Mathematics Research

Abstract Not Available At Time Of Publication.

Abani Patra
DOE Office of Science
abani.patra@science.doe.gov

Steven L. Lee
DOE Office of Science
Advanced Scientific Computing Research
steven.lee@science.doe.gov

MS75
Probabilistic Subspace Clustering and Model Selection for Patch-Based Image Restoration

In this work we propose a patch-based denoising algorithm based on the learning of probabilistic high-dimensional mixture models on the noisy patches. These models take into account the lower intrinsic dimension of each class of the clean patches and the prior is selected among these models using the Bayesian Information Criterion (BIC). The restored image is computed using the conditional expectation knowing this prior and the noise model. This yields a blind denoising algorithm that demonstrates state-of-the-art performance.

Antoine Houdard
LTCI CNRS Télécom ParisTech
antoine.houdard@telecom-paristech.fr

Charles Bouveyron
Universite Paris Descartes
charles.bouveyron@parisdescartes.fr

Julie Delon

Universite Paris Descartes
France
julie.delon@parisdescartes.fr

MS75
Learning Optimally Sparse Image Filters by Quotient Minimisation

Learning approaches have recently become very popular in the field of inverse problems. A large variety of methods has been established in recent years, ranging from bi-level learning to high-dimensional machine learning techniques. Most learning approaches, however, only aim at fitting parametrised models to favourable training data whilst ignoring misfit training data completely. In this talk, we follow up on the idea of learning parametrised regularisation functions by quotient minimisation. We consider one- and higher-dimensional filter functions to be learned and allow for fit- and misfit-training data consisting of multiple functions. We first present results resembling behaviour of well-established derivative-based sparse regularisers like total variation or higher-order total variation in one-dimension. Then, we introduce novel families of non-derivative-based regularisers. This is accomplished by learning favourable scales and geometric properties while at the same time avoiding unfavourable ones.

Carola-Bibiane Schönlieb
DAMTP, University of Cambridge
cbs31@cam.ac.uk

Martin Benning
Institute for Computational and Applied Mathematics
University of Muenster
mb941@cam.ac.uk

Guy Gilboa
Technion Israel Institute of Technology, Israel
guy.gilboa@ee.technion.ac.il

Joana Grah
DAMTP, University of Cambridge
jg704@cam.ac.uk

MS75
Multiscale Regression on Intrinsically Low-dimensional Data

In contemporary science and technology we constantly collect data which, albeit described by a large number of coordinates, feature an underlying low-dimensional structure. Common examples of intrinsic parameters in imaging include pose variations of a scene, facial expressions of a person, and position of lighting sources. Performing learning tasks on such data with good accuracy while maintaining low sample complexity and affordable computational cost turns out to be problematic due to the well known curse of dimensionality. In my talk I will present a universal algorithm to regress response variables on high-dimensional predictors concentrating near sets of (much) lower dimension. Exploring the empirical distribution of the data, we construct piecewise polynomial approximations along a tree of multiscale partitions. Our estimators automatically adapt to the intrinsic geometry of the data, unveiling local features at different levels of detail. We show convergence both in probability and in expectation, providing explicit rates for the finite-sample performance. The rates achieved are optimal (up to logarithmic factors) on a wide

class of priors, and are independent of the ambient dimension. Moreover, the computational cost is $O(n \log n)$, and depends only linearly on the ambient dimension.

Stefano Vigogna, Wenjing Liao, Mauro Maggioni
Johns Hopkins University
svigogna@math.jhu.edu, wliao@math.jhu.edu, mauro@math.jhu.edu

MS75

Low Dimensional Manifold Model for Image Processing

In this talk, I will present a low dimensional manifold model (LDMM) and apply it to image reconstruction problems. LDMM is based on the observation that the patch manifolds of many natural images have low dimensional structure. Based on this fact, the dimension of the patch manifold is used as a regularization to recover the image. The key step in LDMM is to solve a Laplace-Beltrami equation over a point cloud which is solved by the point integral method or weighted graph Laplacian. These two types of discretization enforce the sample point constraints correctly. A semi-local patch distance is used to compute the metric on the patch manifold. Numerical simulations in image processing, hyperspectral imagery reconstruction, and plasma inpainting show that LDMM is a powerful method in reconstruction of noisy and incomplete data.

Zuoqiang Shi
Tsinghua University
zqshi@math.tsinghua.edu.cn

Wei Zhu
Department of Mathematics
University of California, Los Angeles
weizhu731@math.ucla.edu

Stanley J. Osher
University of California
Department of Mathematics
sjo@math.ucla.edu

MS76

Communication Lower Bounds for Matricized-Tensor Times Khatri-Rao Product

The matricized-tensor times Khatri-Rao product (MT-TKRP) computation is the typical bottleneck in algorithms for computing a CANDECOMP/PARAFAC decomposition of a tensor. We will present communication lower bounds for this and related computations on sequential and parallel memory models, and we will discuss the communication costs of existing algorithms for MTTKRP.

Grey Ballard
Wake Forest University
ballard@wfu.edu

Nicholas Knight
New York University
nknight@nyu.edu

Kathryn Rouse
Wake Forest University
rousekm@wfu.edu

MS76

Communication-Avoiding Algorithms: Challenges and New Results

On modern computer architectures, communication, i.e., the movement of data, is much more expensive than floating point operations in terms of time and energy. This is true both in the sequential setting, where communication involves the movement of data between cache levels and main memory, and in the parallel setting, where communication involves sending messages between processors. For algorithms with a low computational complexity, performance can thus be limited by the cost of communication. This has motivated the development of *communication-avoiding* algorithms which reduce or minimize data movement (at perhaps the cost of a small additional amount of computation). In this introductory talk, we present an overview of the current state-of-the-art in the development of communication-avoiding algorithms for both direct and iterative numerical linear algebra. Research in this area requires a three-pronged approach: proving lower bounds on the amount of communication required by an algorithm, designing stable methods that attain those bounds, and developing efficient implementations for particular machines/applications. We touch on work in each of these areas and also discuss major challenges and remaining open problems, with forward references to subsequent talks in this minisymposium.

Erin C. Carson
New York University
erin.carson@nyu.edu

MS76

Matrix Multiplication, a Little Faster

Strassen's matrix multiplication algorithm (1969) was followed by Winograd's (1971) who improved it's complexity by a constant factor. Many asymptotic improvements followed. Yet, they have done so at the cost of large, often gigantic, hidden constants. Consequently, for almost all feasible matrix dimensions Strassen-Winograd's remains the fastest. The leading coefficient of Strassen-Winograd's algorithm was believed to be optimal for matrix multiplication algorithms with 2 2 base case, due to a lower bound of Probert (1976). Surprisingly, we obtain a faster matrix multiplication algorithm, with the same base case size, the same asymptotic complexity, but with a smaller leading coefficient. To this end, we transform the input matrices to a different basis, which can be done fast. We discuss improvements in the communication costs, it's effects on parallelization, and the extension of this method to other Strassen-like algorithms. We also prove a generalization of Probert's lower bound that holds under change of basis. This shows that for matrix multiplication algorithms with a 2 2 base case, the leading coefficient of our algorithm cannot be further reduced, hence optimal.

Oded Schwartz, Elaye E. Karstadt
Hebrew University of Jerusalem
odedsc@cs.huji.ac.il, elaye.karstadt@mail.huji.ac.il

MS76

Communication-Optimal Loop Nests

Communication (data movement) often dominates runtime

and energy costs. We consider the problem of reorganizing loop nests to minimize communication. For loop nests that access array variables subscripted by linear functions of the loop iteration vector, the algebraic relationship between variables and operations leads to communication lower bounds applicable to any reordering of the loop iterations.

Nicholas Knight
New York University
nknight@nyu.edu

MS77

Galerkin Difference Methods for Wave Equations in Two Space Dimensions

In this talk, we discuss the Galerkin Difference (GD) approach to high-order accurate, energy stable discretization of hyperbolic PDE systems. As in classical FEM, the method relies on a framework of Galerkin projection to achieve energy stability. However, in breaking with classical FEM, the scheme obtains high-order accuracy through inclusion of neighboring degrees of freedom rather than degrees of freedom internal to an element. This approach to high-order accuracy is based on ideas from the finite difference community. In higher dimensions, one can construct the method as a tensor product of 1D discretizations, which has the advantage of simplifying multi-dimensional schemes to a series of 1D operators. In this talk, we will emphasis the algebraic properties of tensor products that make this reduction possible. In addition, we will present computational considerations for acoustics and linear elasticity along with numerical results for both.

John Jacangelo, Jeffrey W. Banks
Rensselaer Polytechnic Institute
jacanj@rpi.edu, banksj3@rpi.edu

Thomas M. Hagstrom
Southern Methodist University
Department of Mathematics
thagstrom@smu.edu

MS77

High-Order Finite-Difference Time-Domain Simulation of Electromagnetic Waves at Complex Interfaces Between Dispersive Media

We propose a new numerical scheme for the simulation of electromagnetic waves in linear dispersive media, materials where the permittivity depends on the frequency of the wave. We formulate Maxwell's equations as a second order wave equation with an additional time-history term which is associated with the macroscopic electronic response of the material to the external electric field. This formulation allows us to address material interfaces with complex curvilinear geometries, thereby avoiding the drawbacks of the well-known staggered Yee numerical discretization. We use the physical interface conditions and boundary conditions for Maxwell's equations to develop numerical compatibility conditions which preserve the accuracy and stability of the scheme at the interfaces and boundaries. High accuracy simulation of transient waves at dispersive material interfaces is of particular interest in the fields of plasmonic metamaterials and nano-photonics, with various applications in imaging and sensing.

Michael Jenkinson, Jeffrey W. Banks, William Henshaw
Rensselaer Polytechnic Institute
mikejjenkinson@gmail.com, banksj3@rpi.edu, henshw@rpi.edu

MS77

Scalable Time-Stepping Through Component-Wise Approximation of Matrix Functions

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

Somayyeh Sheikholeslami
The University of Southern Mississippi
s.sheikholeslami@usm.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS77

Improving Boundary Derivative Recovery in Elliptic PDEs

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 postprocessing: 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.

David Wells
Rensselaer Polytechnic Institute
wellsd2@rpi.edu

MS78

The Curvature-Dependent Surface Stress Model and Its Effects on the Overall Properties of Nano-Composites

Experiments and materials simulation have demonstrated the curvature-dependence of surface energy and surface stress. Based on these findings, a curvature-dependent surface stress model is developed, which fully considers the curvature effect of surface energy and the initial stress field induced by residual surface stress in the bulk body. Both the finite deformation theory and linear small-deformation theory are provided. First, a curvature-dependent surface energy formula is proposed. It has simple forms and clear physical meanings. Next, the surface constitutive relations are derived, which could predict the size effect of surface tension and agrees well with the atomistic simulation. Then, the surface equilibrium equation is given, which accounts for the internal flexural resistance of the

surface. The above results show the significance of residual surface stress and suggest that it is advantageous and convenient to use the Lagrangian description of the surface fundamental equations to consider the surface effect. Finally, the present theory is applied to study the effective properties of nano-structured materials. A micromechanics framework is proposed to consider both the surface stress effect and the particle size distribution. The numerical results indicate that the curvature effect causes a much stronger size dependence of the effective modulus and the influence of particle size distribution becomes obvious when the dispersion of the particle radius is large.

Xiang Gao
Tufts University
USA
victor.gaox@gmail.com

MS78

Theoretical and Computational Aspects of Thermo-mechanical Solids with Energetic Material Interfaces with Application to Nano-materials

Abstract Not Available At Time Of Publication.

Stefan Kaessmair
University of ErlangenNuremberg, Germany
stefan.kaessmair@ltm.uni-erlangen.de

Ali Javili
Bilkent University
ajavili@bilkent.edu.tr

Paul Steinmann
Chair of Applied Mechanics
Friedrich-Alexander-University Erlangen-Nuremberg
paul.steinmann@ltm.uni-erlangen.de

MS78

Stress Concentrations around Nanovoids and Nanoinhomogeneities

Stress concentration is one of the major challenges threatening the health and integrity of engineering structures. In this talk, we analyze the stress distributions around spherical nanovoids and nanoinhomogeneities near domain boundaries. The loading considered in our analysis includes all-around tension, uniaxial tension, and pure shear, all uniformly applied at infinity. Flat boundaries of the elastic substrates assume traction free boundary conditions whereas the spherical void surface is modeled as a mathematical thin-film of Gurtin and Murdoch type. The method of Boussinesq's displacement functions is used in the analysis and the solutions are typically expressed semi-analytically in terms of infinite series of Legendre functions and improper integrals involving Bessel functions. Numerical calculations are performed to illustrate the dependence of elastic fields on surface material properties, model size, void radius, as well as eccentricity, if applicable. The results suggest the likelihood of optimizing stress concentrations in a variety of materials and structures by the proper design of surface material properties, namely the residual surface stress and the surface Lame constants.

Changwen Mi
Southeast University
China
mi@seu.edu.cn

Demitris Kouris
Office of the Provost
South Dakota School of Mines & Technology
demitris.kouris@sdsmt.edu

MS78

Liquid Inclusions in Soft Materials Capillary Effect, Mechanical Stiffening and Enhanced Electromechanical Response

Abstract Not Available At Time Of Publication.

Pradeep Sharma
University of Houston
USA
psharma@central.uh.edu

MS79

Sampling, Polynomial Chaos and Function Trains Multilevel/Multifidelity Strategies for Forward UQ

In recent years a considerable effort has been devoted to multifidelity approaches in order to pursue a cost reduction for forward UQ analysis. A particular family of multifidelity techniques is the so-called multilevel approach in which the lower fidelity models are coarse representations of the solution. Previous studies demonstrated that the possible combination of both resolution levels and model fidelities can lead to additional cost reduction. In this talk we present a comparison between two families of approaches, namely sampling methods (Monte Carlo, multilevel MC and multilevel-multifidelity MC) and polynomial expansions (compressed sampling Polynomial Chaos and Function Trains) reformulated in a multilevel and/or multifidelity fashion. We aim to highlight advantages and disadvantage of each technique for a collection of moderate to high-dimensional problems. The set of test cases spans simplified model problems to realistic engineering applications including, for instance, a nozzle engine thermo-structural-analysis and a performance estimation for a supersonic combustion (scramjet) engine.

Gianluca Geraci
Sandia National Laboratories, NM
ggeraci@sandia.gov

Alex A. Gorodetsky
Massachussets Institute of Technology
goroda@mit.edu

John D. Jakeman
Sandia National Labs
jdjakem@sandia.gov

Michael S. Eldred
Sandia National Laboratories
Optimization and Uncertainty Quantification Dept.
mseldre@sandia.gov

MS79

A Bi-Fidelity, Low-Rank Approximation Technique for Uncertainty Quantification

The use of model reduction has become widespread as a means to reduce computational cost for uncertainty quantification of PDE systems. In this work we present a model reduction technique that exploits the low-rank structure of the solution of interest, when it exists, for fast propagation

of high-dimensional uncertainties. To construct this low-rank approximation, the proposed method utilizes models with lower fidelities (hence cheaper to simulate) than the intended high-fidelity model. After obtaining realizations to the lower fidelity models, a reduced basis and an interpolation rule are identified and applied to a small set of high-fidelity realizations to obtain this low-rank, bi-fidelity approximation. In addition to the construction of this bi-fidelity approximation, we present convergence analysis and numerical results.

Jerrad Hampton
University of Colorado, Boulder
jerrad.hampton@colorado.edu

Hillary Fairbanks
Department of Applied Mathematics
University of Colorado, Boulder
hillary.fairbanks@colorado.edu

Alireza Doostan
Department of Aerospace Engineering Sciences
University of Colorado, Boulder
Alireza.Doostan@Colorado.EDU

Akil Narayan
University of Utah
akil@sci.utah.edu

MS79

Optimization of Random Systems Using Multi-Fidelity Models

Abstract Not Available At Time Of Publication.

Phaedon-Stelios Koutsourelakis
Technische Universität München
Germany
p.s.koutsourelakis@tum.de

Maximilian Koschade
Technical University of Munich
maximilian.koschade@tum.de

MS79

Deep Multi-Fidelity Gaussian Processes

Abstract Not Available At Time Of Publication.

Maziar Raissi, George Em Karniadakis
Brown University
maziar_raissi@brown.edu, george_karniadakis@brown.edu

MS80

Kristin Bennett

In this panel, we consider effective ways to modify the mathematics curriculum to better train future data scientists.

Kristin Bennett
Mathematical Sciences
Rensselaer Polytechnic Institute
bennek@rpi.edu

MS80

Randy Paffenroth

In this panel, we consider effective ways to modify the mathematics curriculum to better train future data scientists.

Randy Paffenroth
Worcester Polytechnic Institute
rcpaffenroth@wpi.edu

MS80

Louis Rossi

In this panel, we consider effective ways to modify the mathematics curriculum to better train future data scientists.

Louis Rossi
University of Delaware
rossi@udel.edu

MS81

Diffusion Based Metrics for Naturally Occuring Networks: Background and Applications

Abstract Not Available At Time Of Publication.

Lenore J. Cowen
Dept. of Computer Science
Tufts University
lenore.cowen@tufts.edu

MS81

Algebraic Multilevel Methods for Computing Diffusion-based Metrics on Graphs

Recently, diffusion-based metrics have been developed for protein-protein interaction networks and used for protein function prediction. In this talk, we focus on the challenges in computing these diffusion-based metrics, especially for large-scale networks. By exploring the algebraic properties of the distance metrics, we reformulate the computation of distances into solving a series of graph Laplacians systems. In particular, we develop algebraic multilevel methods for solving the resulting linear systems efficiently. Applications to the protein-protein networks will be presented and possible generalizations will be discussed

Junyuan Lin, Xiaozhe Hu
Tufts University
junyuan.lin@tufts.edu, xiaozhe.hu@tufts.edu

Lenore J. Cowen
Dept. of Computer Science
Tufts University
lenore.cowen@tufts.edu

MS81

Optimal Target Sets for a Random Walk On a Finite Graph

Motivated by the problem of finding optimal spreaders and optimal targets in networks, we study a combinatorial optimization problem that arises from a random walk on a

graph G. The graph can be directed or undirected. Given A a subset of vertices, we define the set function $F(A)$ to be the sum of the first hitting times to A by random walkers that start at nodes outside of A. Suppose we fix the cardinality to be K, then A is optimal if it minimizes $F(A)$ over all sets of size K. Identifying such a set is probably NP hard but fortunately F is supermodular and non-increasing. We present a new proof of these facts using a first hitting time representation of the increments of F. We will show the relationship between this problem in the undirected graph case and other optimization problems such as finding a partial vertex cover and minimum dominating set for G. Unlike the deterministic objective functions used there, F also involves the occupation time of a random walker in the complement set before reaching A. We discuss an approach to obtaining upper bounds on F that uses the deterministic upper bounds and upper bounds on the occupation time. Effective upper bounds can be used to identify optimal and near optimal sets for our problem.

Fern Y. Hunt
National Institute of Standards and Technology
fern.hunt@nist.gov

MS82
Isogeometric Analysis and Hierarchical T-splines

High precision numerical results depend strongly upon both the ability to perform highly accurate numerical calculations *and* the ability to accurately represent the geometry of the underlying problem. Isogeometric analysis merges these two goals by using a common basis for both design and analysis. Most of the initial isogeometric analysis technique used non-uniform rational B-splines; however, newer bases such as T-splines have shown great promise in accurately representing geometries without some of the difficulties associated with B-splines. To more effectively use T-splines for analysis we have developed a hierarchical technique that allows us to solve problems with high precision efficiently. In this talk, we will introduce the ideas behind isogeometric analysis, T-splines and also present the hierarchical technique for T-splines.

Emily Evans
Mathematics Department
Brigham Young University
ejevans@math.byu.edu

MS82
Computationally-Inferred Numerical Wave Numbers with Applications to Non Uniform Meshes

It is well-known that errors in modified wave number and modified temporal amplification factor, or modified frequency, lead to numerical dispersion and dissipation errors. In this presentation, we try to answer the question, that given a numerical solution of the convective wave equation, how well can we recover the modified wave number and modified frequency of the spatial schemes? While a regular Fourier analysis in space or time assumes a uniform mesh, the computationally inferred modified wave number and modified frequency can be applied to nonuniform meshes. The essential formulas for finding computationally inferred modified wave number and frequency are given. Validation examples with known analytical results are presented and discussed. Applications to wave propagation on nonuniform meshes, where analytical expressions for modified wave number and modified frequency are difficult to find, are also presented, in one dimension and two dimen-

sions. As computational meshes in practical applications become increasingly nonuniform and unstructured, and the numerical algorithms increasing adaptive, methods such as the one presented in this paper that can provide quantitative assessment of numerical dispersion and dissipation errors for these schemes are increasingly needed.

Anne M. Fernando
Norfolk State University
Norfolk State University
amfernando@nsu.edu

MS82
Modeling Intermittent Preventative Treatment and Drug Resistance in Malaria

An age-structured ODE model is presented to investigate the role of Intermittent Preventive Treatment (IPT) in averting malaria-induced mortality in children, and its related cost in promoting the spread of anti-malarial drug resistance. IPT, a malaria control strategy in which a full curative dose of an antimalarial medication is administered to vulnerable asymptomatic individuals at specified intervals, has been shown to reduce malaria transmission and deaths in children and pregnant women. It can also promote drug resistance spread. Our mathematical model is used to explore IPT effects on drug resistance and deaths averted in holoendemic malaria regions. The model includes drug-sensitive and drug-resistant strains as well as human hosts and mosquitoes. The basic reproduction and invasion reproduction numbers for both strains are derived. Numerical simulations include individual and combined effects of IPT and treatment of symptomatic infections on the prevalence of both strains and the number of lives saved. Our results suggest that while IPT can indeed save lives, particularly in high transmission regions, certain combinations of drugs used for IPT and to treat symptomatic infection may result in more deaths when resistant parasite strains are circulating. A sensitivity analysis indicates outcomes are most sensitive to the reduction factor of transmission for the resistant strain, rate of immunity loss, and the natural clearance rate of sensitive infections.

Carrie A. Manore
Los Alamos National Laboratory
cmanore@lanl.gov

MS82
Inclusion of Asymptotic Individuals to Model Influenza Transmission

The age-structure model SAIQR is presented, where S (susceptible), A (Asymptomatic), I (Infectious), Q (Quarantine) and R (Recovered) individuals are included. The inclusion of the asymptomatic class makes the age-structure SIQR model more accurate for the dynamics transmission of Influenza. In this work a system of partial differential equations is used to model this dynamics. An explicit analytic expression was attained for the endemic steady state solution, as well as an analytic expression for the Reproduction Number, which allows to execute numerical simulations, and to identify the relevant parameters during influenza transmission.

Ana Vivas Barber
Norfolk State University

alvivasbarber@nsu,edu

MS83
Optimal Sampling for Recovering Sparse and Compressible Orthogonal Polynomial Expansions

We propose a novel sampling and weighting scheme for recovery of compressible multivariate polynomial chaos expansions. When the orthogonal basis stems from a tensorial measure, then proposed method has uniform optimal recovery properties for any multi-index set. The algorithmic procedure involves sampling from measures that are "induced" by univariate measures. We present recovery examples for a variety of tensorial measures and multi-index sets that showcase the efficacy of the procedure.

Akil Narayan
University of Utah
akil@sci.utah.edu

MS83
High-dimensional Function Interpolation with Gradient-enhanced Weighted ℓ_1 Minimization

Many physical problems involve in approximating high-dimensional functions with a limited number of sampling points. It is seen that the high-dimensional function interpolation problem has various applications such as uncertainty quantification. For example, in order to compute a quantity of interest for the parametric PDE, high-dimensional function approximation is often required. In this talk, we present the work of interpolating a high-dimensional function using the weighted ℓ_1 minimization technique when both points for the original function and its derivatives are sampled. With additional derivative information, we see a numerical improvement over the case only samples points from the original function. A theoretical analysis for this interpolation problem with derivative information incorporated is also presented.

Yi Sui, Ben Adcock
Simon Fraser University
ysui@sfu.ca, ben_adcock@sfu.ca

MS83
Sparse Optimization in Learning Governing Equations for Time-Varying Measurements

Learning the governing equations for time-varying measurement data is of great interest across different scientific fields.Recovering the governing equations becomes quite challenging, when such data is moreover highly corrupted, or does not hold certain properties. In this work, we show how to utilize compressed sensing strategy to identify the underlying nonlinear differential equations. Theoretical reconstruction guarantee as well as various numerical experiments will be presented.

Giang Tran
The University of Texas at Austin
gtran@math.utexas.edu

MS83
Unified Sufficient Conditions for Uniform Recovery of Sparse Signals via Nonconvex Minimizations

Nonconvex minimizations are generally closer to ℓ_0 penalty than ℓ_1 norm, thus it is widely accepted that they are able to enhance the sparsity of the solutions. The theory verifying that nonconvex penalties are as good as or better than ℓ_1 minimization in exact, uniform recovery of sparse signals, however, has not been available beyond a few specific cases. We aim to fill this gap by establishing recovery guarantees through unified null space properties that encompass most currently proposed nonconvex functionals in the literature. These conditions are less demanding than or identical to the standard null space property, the necessary and sufficient condition for ℓ_1 minimization.

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

Hoang A. Tran
Oak Ridge National Laboratory
Computer Science and Mathematics Division
tranha@ornl.gov

MS84
Transmission Models and Management of Lymphatic Filariasis Elimination

Abstract Not Available At Time Of Publication.

Edwin Michael
University of Notre Dame
edwin.michael.18@nd.edu

MS84
Modeling Infection Transmission Dynamics and Elimination of Leishmaniasis

Abstract Not Available At Time Of Publication.

Anuj Mubayi
Arizona State University
amubayi@asu.edu

MS84
Leading Indicators for Anticipating Elimination of Mosquito-Borne Diseases

Mosquito-borne diseases contribute significantly to the global disease burden. High-profile elimination campaigns are currently underway for many parasites, e.g., Plasmodium spp., the causal agent of malaria. Sustaining momentum near the end of elimination programs is often difficult to achieve and consequently quantitative tools that enable monitoring the effectiveness of elimination activities after the initial reduction of cases has occurred are needed. In this talk, I consider compartmental Ross-McDonald models that are slowly forced through a critical transition through gradually deployed control measures. I derive expressions for the behavior of candidate indicator statistics, including the autocorrelation coefficient, variance, and coefficient of variation in the number of human cases during the approach to elimination. We conducted a simulation study to test the performance of each summary statistic as an early warning system of mosquito-borne disease elimination. Variance and coefficient of variation were highly predictive of elimination but autocorrelation performed poorly as an indicator in some control contexts. Our results suggest that bifurcations in mosquito-borne infectious disease systems may be foreshadowed by characteristic temporal patterns of disease prevalence.

Suzanne M. O'Regan

North Carolina A&T State University
smoregan@ncat.edu

Jonathan Lillie
North Hall High School, GA
jonathan.lillie@gmail.com

John M. Drake
University of Georgia
jdrake@uga.edu

MS84

Evaluating Long-Term Effectiveness of Sleeping Sickness Control Measures in Guinea

Abstract Not Available At Time Of Publication.

Abhishek Pandey
Department of Biostatistics, Yale University
abhishek.pandey@yale.edu

MS85

Low-Rank Matrix Reconstruction: Algorithms and Theory

In this talk, we discuss the problem of how to recover a low rank matrix from its limited information, which arises from many practical applications in machine learning, imaging, signal processing, computer vision, etc. Typically, the low rank matrix to be recovered is of a large scale and the number of linear measurements is small. We will introduce both convex and non-convex algorithms, and theory on the guarantee of their convergence to the correct low-rank matrix.

Jian-Feng Cai
Department of Mathematics
Hong Kong University of Science and Technology
jfcai@ust.hk

MS85

Communication Avoiding Primal and Dual Block Coordinate Descent Methods

Primal and dual block coordinate descent are iterative methods for solving regularized and unregularized optimization problems. Distributed-memory parallel implementations of these methods have become popular in analyzing large machine learning datasets. However, existing implementations communicate at every iteration which, on modern data center and supercomputing architectures, often dominates the cost of floating-point computation. We evaluate the performance of new communication-avoiding variants of the primal and dual block coordinate descent for regularized least squares.We test our communication-avoiding algorithms on dense and sparse datasets (both synthetic and real) to illustrate the speedups attainable on a Cray XC30 supercomputer. We evaluate the strong and weak scaling performance on up to 6144 cores to illustrate the speedups attainable.

Kimon Fountoulakis, Aditya Devarakonda, James Demmel, Michael Mahoney
UC Berkeley
kfount@berkeley.edu, aditya@eecs.berkeley.edu, dem-mel@eecs.berkeley.edu, mmahoney@stat.berkeley.edu

MS85

Approximate Least-Squares-Based Methods for Efficient Learning

Abstract: Two approximate algorithms based on least squares that accelerate classical machine learning methods will be presented. The first is about interpolating Cholesky factors for efficient cross validation in ridge regression; the second is an approximate way to compute Locally Linear Coding in image classification, which we call hardware-compliant image encoding and exploits the efficiency of BLAS-3 level operations. The proposed algorithms can typically achieve a speedup factor of 5 and 40, respectively, without sacrificing quality.

Da Kuang
University of California, Los Angeles
dakuang@math.ucla.edu

Alex Gittens
UC Berkeley
gittens@icsi.berkeley.edu

Raffay Hamid
DigitalGlobe Inc
raffay@gmail.com

MS85

Fast Spatial Gaussian Process Maximum Likelihood Estimation Via Skeletonization Factorizations

Maximum likelihood estimation for parameter-fitting given observations from a kernelized Gaussian process in space is a computationally-demanding task that restricts the use of such methods to moderately-sized datasets. We present a procedure for unstructured 2D observations that allows for evaluation of the log-likelihood and its gradient (i.e., the score equations) in $\mathcal{O}(n^{3/2})$ time and $\mathcal{O}(n \log n)$ storage, where n is the number of observations. Our method relies on the skeletonization procedure described by Martinsson & Rokhlin (2005) in the form of the *recursive skeletonization factorization* of Ho & Ying (2015). Combining this with an adaptation of the matrix peeling algorithm of Lin et al. (2011), our method can be used in the context of any first-order optimization routine to quickly and accurately compute maximum-likelihood estimates.

Victor Minden, Anil Damle, Ken Ho
Stanford University
vminden@stanford.edu, asd239@cornell.edu,
klho@stanford.edu

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS87

A Multigrid Perspective on the Parallel Full Approximation Scheme in Space and Time

For the numerical solution of time-dependent partial differential equations, time-parallel methods have recently shown to provide a promising way to extend prevailing strong-scaling limits of numerical codes. One of the most

complex methods in this field is the "Parallel Full Approximation Scheme in Space and Time' (PFASST). PFASST already shows promising results for many use cases and many more is work in progress. However, a solid and reliable mathematical foundation is still missing. We show that under certain assumptions the PFASST algorithm can be conveniently and rigorously described as a multigrid-in-time method. Following this equivalence, first steps towards a comprehensive analysis of PFASST using blockwise local Fourier analysis are taken. The theoretical results are applied to examples of diffusive and advective type.

Matthias Bolten
University of Wuppertal
Germany
bolten@math.uni-wuppertal.de

Dieter Moser
Juelich Supercomputing Centre
Forschungszentrum Juelich
d.moser@fz-juelich.de

Robert Speck
Juelich Supercomputing Centre
Forschungszentrum Juelich GmbH
r.speck@fz-juelich.de

MS87
Multigrid Reduction in Time Applied to 1D Hyperbolic Problems

The current trend in computer architectures is towards greater numbers of processors with little improvement in clock speeds, hence future computational speedups must be obtained through algorithms with greater concurrency. In such a situation sequential time stepping is a clear computational bottleneck due to the lack of parallelism in the time dimension. We consider the multigrid reduction in time (MGRIT) algorithm, an iterative procedure which uses multigrid reduction techniques and a multilevel hierarchy of coarse time grids to allow temporal parallelism. In this talk, we discuss how to use spatial coarsening as well as temporal coarsening in constructing the hierarchy of grids for MGRIT applied to 1D hyperbolic partial differential equations. In the case of explicit time stepping, spatial coarsening may be necessary to ensure that stability conditions are satisfied on all levels, and it may be useful for implicit time stepping by producing cheaper multigrid cycles. Unfortunately, classical spatial coarsening results in extremely slow convergence when the wave speed is near zero, even if only locally. We present an adaptive spatial coarsening strategy that addresses this issue for 1D linear advection with variable wave speed. Numerical results show that this offers significant improvements over classical coarsening.

Alexander Howse
University of Waterloo
ajmhowse@gmail.com

MS87
Towards Better Scalability in the Parareal in Time Algorithm

Among the methods to parallelize the solution of PDEs, the decomposition of the time domain stands still today only as a secondary choice. This is due to intrinsic limitations in the optimal parallel efficiency that the existing methods can deliver. In this talk, we address this obstruction in the case of the parareal in time algorithm. The method is iterative and its efficiency limitations come from the repeated use of a high resolution solver at all steps. An idea that has been successfully tested in previous works is to compute inexact but cheaper realizations of this accurate solver which are built using information from previous steps. In this talk, we will give a theoretical framework for the rigorous convergence analysis of this strategy. We will also discuss the evaluation of the gain in efficiency and illustrate our statements with numerical examples.

Yvon Maday
Universite Pierre et Marie Curie
and Brown university
maday@ann.jussieu.fr

Olga Mula
CEREMADE (Paris Dauphine University)
mula@ceremade.dauphine.fr

Walid Kheriji
Universite Pierre et Marie Curie and CEA
kheriji.walid@gmail.com

MS87
Waveform Relaxation with Adaptive Pipelining

Instead of discretizing first in time and solving the resulting sequence of spatial PDEs by domain decomposition, one can first decompose in space and consider each subdomain problem as an independent space-time problem. Enforcing consistency results in a sequence of space-time problems to be solved on each spatial subdomain. This approach is known as waveform relaxation, and the sequence of space-time problems are referred to as waveform iterates. Waveform relaxation provides flexibility in the choice of spatial and temporal grids and integrators. Additionally, multiple waveform iterates can be simultaneously computed in a pipeline fashion. In this work, are are interested in adaptively choosing the number of waveform iterates at each time step. We provide some numerical evidence that supports one's intuition about the proposed Waveform Relaxation method with Adaptive Pipelining (WRAP), followed by an analysis of the convergence and # of iterations for the WRAP method applied to the homogeneous heat equation.

Benjamin W. Ong
Michigan Technological University
ongbw@mtu.edu

Felix Kwok
Hong Kong Baptist University
felix_kwok@hkbu.edu.hk

MS88
The Triangle Free Process

Abstract Not Available At Time Of Publication.

Thomas Bohman
Carnegie-Mellon

tbohman@math.cmu.edu

MS88
Increasing Sequences of Integer Triples

We will consider the following deceptively simple question, formulated recently by Po-Shen Loh. Define the '2-less than' relation on the set of triples of integers by saying that a triple x is 2-less than a triple y if x is less than y in at least two coordinates. What is the maximal length of a sequence of triples taking values in $\{1, ..., n\}$ which is totally ordered by the '2-less than' relation? In his work, Loh uses the triangle removal lemma to improve slightly on the trivial upper bound of n^2, and conjectures that the truth should be of order $n^{3/2}$. The gap between these bounds has proved to be surprisingly resistant. We shall discuss joint work with Tim Gowers, giving some developments towards this conjecture and a wide array of natural extensions of the problem, many of which remain open.

Jason Long
Cambridge
Cambridge (U.K.)
jl694@cam.ac.uk

MS88
Abelian Sandpiles

Abstract Not Available At Time Of Publication.

Wes Pegden
Carnegie-Mellon
wes@math.cmu.edu

MS89
Extremely Scalable Finite Element Solvers for Turbulent Incompressible Flows Through Segregated Runge-Kutta Schemes

We propose a framework for the High Performance Computing (HPC) of turbulent incompressible flows that relies on the extreme scalability of Balancing Domain Decomposition by Constraints (BDDC) preconditioners. We use a Large Eddy Simulation (LES) technique based on the Variational MultiScale (VMS) method, which has been shown to give accurate results, see "[O. Colomés, S. Badia, R. Codina, J. Principe, Assessment of variational multiscale models for the large eddy simulation of turbulent incompressible flows, Computer Methods in Applied Mechanics and Engineering, 285 (2015) 32-63]". To tackle the time integration we use the Segregated Runge-Kutta (SRK) schemes, firstly proposed in "[O. Colomés, S. Badia, Segregated Runge-Kutta methods for the incompressible Navier-Stokes equations, International Journal for Numerical Methods in Engineering, 105(5) (2016) 372-400]", which are based on two main goals: velocity-pressure segregation and preservation of the same order of accuracy for both fields. Our approach to reach extremely scalable FE solvers is to consider SRK time integration schemes, with a VMS method acting as an LES method, and using BDDC preconditioners to reach extreme scalability. This approach was described in "[O. Colomés, S. Badia, Segregated Runge-Kutta time integration of convection-stabilized mixed finite element schemes for wall-unresolved LES of incompressible flows, Computer Methods in Applied Mechanics and Engineering, 313 (2017) 189-215]".

Oriol Colomes

Duke University
oriol.colomes@duke.edu

Santiago Badia
Universitat Politecnica de Catalunya, Spain
sbadia@cimne.upc.edu

MS89
Large Eddy Simulation Reduced Order Models

This talk proposes several large eddy simulation reduced order models (LES-ROMs) based on proper orthogonal decomposition (POD). To develop these models, explicit POD spatial filtering is introduced. Two types of spatial filters are considered: A POD projection onto a POD subspace and a POD differential filter. These explicit POD spatial filters allow the development of two types of ROM closure models: phenomenological and approximate deconvolution. Furthermore, the explicit POD spatial filters are used to develop regularized ROMs in which various ROM terms are smoothed (regularized). The new LES-ROMs are tested in the numerical simulation of a three-dimensional flow past a circular cylinder at a Reynolds number $Re = 1000$.

Traian Iliescu
Department of Mathematics
Virginia Tech
iliescu@vt.edu

Xuping Xie
Virginia Tech
xupingxy@vt.edu

MS89
Computation of Sensitivity and Stability in Chaotic Flow

Abstract Not Available At Time Of Publication.

Qiqi Wang
Massachusetts Institute of Technology
qiqi@mit.edu

MS90
Lddmm Models of a Heartbeat

While LDDMM methods and algorithms have proven their worth when comparing macroscopic differences between organs, it is ill-suited to generate a heartbeat, which requires a torsion in the muscle that does not naturally appear through shape matching. In this talk, we show various possible models to generate a heartbeat from a relaxed state to a contracted state while in the framework of LDDMMs, using for example constraints or artificially generated fibers, and their success (or lack of success) in modeling a heartbeat while keeping computations to a manageable level.

Sylvain Arguillere
CNRS
Institut Camille Jordan
arguillere@math.univ-lyon1.fr

MS90
Higher Order Sobolev Metrics for Shape Optimiza-

tion and Shape Matching

Statistical shape analysis can be done in a Riemannian framework by endowing the set of shapes with a Riemannian metric. Sobolev metrics of order two and higher on shape spaces of parametrized or unparametrized curves have several desirable properties not present in lower order metrics, but their discretization is still largely missing. We present algorithms to numerically solve the geodesic initial and boundary value problems for these metrics. The combination of these algorithms enables one to compute Karcher means in a Riemannian gradient-based optimization scheme and perform principal component analysis and clustering. Our framework is sufficiently general to be applicable to a wide class of metrics. We demonstrate the effectiveness of our approach by analyzing a collection of shapes representing HeLa cell nuclei.

Martin Bauer
Florida State University
bauer@math.fsu.edu

Nicolas Charon
Center for Imaging Sciences
Johns Hopkins University
charon@cis.jhu.edu

MS90

A New Method for Comparing Closed Surfaces in $\mathbb{R}^3$

In this talk we describe a new method of putting a metric on the space of closed surfaces in $\mathbb{R}^3$ modulo reparametrization, and show some results of its implementation.

Eric Klassen
Florida State University
klassen@math.fsu.edu

MS90

Diffeomorphic Models for Curve and Surface Comparison

We consider the results of combining two approaches developed for the design of Riemannian metrics on curves and surfaces, namely parametrization-invariant metrics of the Sobolev type on spaces of immersions, and metrics derived through Riemannian submersions from right-invariant Sobolev metrics on groups of diffeomorphisms (the latter leading to the large deformation diffeomorphic metric mapping framework). While these metrics, which were enumerated and studied in the case of curves in a 2007 paper by P. Michor and D. Mumford, can easily be combined in theory, very little effort has been dedicated towards doing so for practical applications. In this talk, we will illustrate the increased modeling flexibility resulting from using hybrid metrics, especially when comparing arrangements of multiple curves and surfaces.

Laurent Younes
Center for Imaging Science
Johns Hopkins University
laurent.younes@jhu.edu

MS91

The Cauchy Problem for the Quantum Boltzmann Equation for Bosons at Very Low Temperature

Abstract Not Available At Time Of Publication.

Ricardo Alonso
Department of Mathematics
PUC-Rio
ricardoalonsoplata@gmai.com

MS91

Convergence of Discrete Minimizers to Continuum Minimizers for the Interaction Energy

Under suitable technical conditions we show that minimizers of the discrete interaction energy for attractive-repulsive potentials converge to minimizers of the corresponding continuum energy as the number of particles goes to infinity. We prove that the discrete interaction energy Gamma-converges in the weak topology to the continuum interaction energy. As part of the proof we study regularity properties of minimizers: we show that continuum minimizers belong to suitable Morrey spaces and we introduce the set of empirical Morrey measures as a natural discrete analog containing all the discrete minimizers. This is joint work with José Alfredo Cañizo.

Francesco Patacchini
Imperial College London
f.patacchini13@imperial.ac.uk

MS91

Euler-Alignment System with Nonlinear Fractional Dissipation

Abstract Not Available At Time Of Publication.

Changhui Tan
Rice University
ctan@rice.edu

MS91

Fractional Diffusion Limit for E.COLI Chemotaxis

Abstract Not Available At Time Of Publication.

Min Tang
Shanghai Jiao Tong University, Department of Math
China
tangmin@sjtu.edu.cn

MS92

Design of Optimal Experiments for Compressive Sampling of Polynomial Chaos Expansions: Application to Uncertainty Quantification

Surrogate modeling is the process of constructing a computationally cheap, approximate model of an unknown quantity of interest (QoI), as a function of model inputs. In the context of uncertainty quantification, polynomial chaos expansions (PCEs) are basis representations that are frequently used to construct surrogate models for complex problems, where model inputs are uncertain. Many PCEs of engineering QoIs admit sparse approximations, for which compressive sampling techniques that exploit this sparsity provide a natural approximation framework. We propose a novel compressive sampling approach based on the classical design of optimal experiments framework, where the realizations of the QoI are generated via a deterministic

instead of a standard random sampling scheme. We then demonstrate the effectiveness of the approach to PCEs of sparse QoIs, either manufactured or associated with the solution of parametric PDEs, and compare our sampling strategy to those using random samples.

Paul Diaz
University of Colorado, Boulder
paul.diaz@colorado.edu

Alireza Doostan
Department of Aerospace Engineering Sciences
University of Colorado, Boulder
Alireza.Doostan@Colorado.EDU

MS92

Lebesgue Constants for Weighted Leja Sequences on Unbounded Domains

The standard Leja points are a nested sequence of points defined on a compact subset of the real line, and can be extended to unbounded domains with the introduction of a weight function $w : R \to [0, 1]$. Due to a simple recursive formulation, such abcissas show promise as a foundation for high-dimensional approximation methods such as sparse grid collocation, deterministic least squares, and compressed sensing. Just as in the unweighted case of interpolation on a compact domain, we use results from potential theory to prove that the Lebesgue constant for the Leja points grows subexponentially with the number of interpolation nodes.

Peter Jantsch
University of Tennessee, Knoxville
Department of Mathematics
pjantsch@vols.utk.edu

MS92

Global Reconstruction of Solutions to Parameterized PDEs via Compressed Sensing

We propose and analyze a novel compressed sensing-based polynomial approximation for PDEs with stochastic and parametric inputs. Unlike standard compressed sensing techniques which only approximate functionals of parameterized solutions, e.g., evaluation at a single spatial location, we consider an L1-regularized problem involving Hilbert-valued signals, i.e., signals where each coordinate is a function belonging to a Hilbert space, which provide a direct, global reconstruction of the solutions in the entire physical domains. The advantages of our approach over the pointwise recovery with standard techniques include: i) for many parametric and stochastic model problems, global estimates of solutions in the physical domain are quantities of interest; ii) the recovery guarantees of our strategy can be derived from the decay of the polynomial coefficients in the relevant functional space, which is well known in the existing theory; and iii) the global reconstruction only assumes a priori bounds of the tail expansion in energy norms, which are much more realistic than pointwise bounds. We perform extensive numerical experiments on several high-dimensional parameterized elliptic PDE models to demonstrate the superior recovery property of the proposed approach. Combining with some recently developed strategies, its effectiveness can be further enhanced, numerical results emphasizing this fact are also presented.

Hoang A. Tran

Oak Ridge National Laboratory
Computer Science and Mathematics Division
tranha@ornl.gov

Nick Dexter
University of Tennessee
ndexter@utk.edu

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

MS93

Black-box Communication Optimal Low Rank Approximations

In this talk we shall present a black-box QR based algorithm and its parallel implementation for computing a low-rank approximation of matrices arising from boundary element problems. Our algorithm is black-box in the sense that the evaluation of pairwise interactions does not rely on any analytic expansion, but only relies on the entries and the hierarchical structure of the matrix. This new method shows good performance when compared to other existing methods such as the Adaptive Cross Approximation, Fast Multipole Method and the approaches based on singular value decompositions. Our approach has the advantage of being based on a stable QR factorization, requiring linear cost and optimal communication cost when performed in parallel on large scale computers.

Alan Ayala
Inria
alan.ayala-obregon@inria.fr

Xavier Claeys
Paris 6 - LJLL
claeys@ann.jussieu.fr

Laura Grigori
INRIA
France
Laura.Grigori@inria.fr

MS93

Communication-Avoiding Primal and Dual Methods for Regularized Least-Squares

We build on existing work on communication-avoiding Krylov subspace methods by extending those results to machine learning where scalable algorithms are especially important given the enormous amount of data. Block coordinate descent methods are routinely used in machine learning to solve optimization problems. Given an $m \times n$ matrix X where the rows are features of the data and the columns are samples, block coordinate descent methods can compute the regularized or unregularized least squares solution by iteratively solving a subproblem using a block of b rows of X. This process is repeated until the solution converges to the desired accuracy or until the number of iterations has reached a user-defined limit. This suggests that, if the matrix is partitioned across some number of processors then the algorithm communicates at each iteration in order to solve the subproblem. This follows from the fact that the primal method uses b features (resp. samples for the dual method) and computes a Gram matrix. The running time for such methods is often dominated by communication cost which increases with the number of

processors (P). In contrast to other results such as CoCoA and HogWILD! , our results reduce the latency cost in the primal and dual block coordinate descent methods by a factor of s, a tuning parameter, on distributed-memory architectures without changing the convergence behavior, in exact arithmetic.

Aditya Devarakonda, Kimon Fountoulakis, James Demmel, Michael Mahoney
UC Berkeley
aditya@eecs.berkeley.edu, kfount@berkeley.edu, demmel@eecs.berkeley.edu, mmahoney@stat.berkeley.edu

MS93
Communication-Avoiding Sparse Inverse Covariance Matrix Estimation

Sparse inverse covariance matrix (ICM) estimation is a common problem in statistics and machine learning. It unveils the graphical model behind observed variables and can be used to analyze data in many fields. Because of its high computational complexity, there are few implementations that support more than tens of thousands of variables. Our work enables, for the first time, analyzing high-dimensional data sets with millions of variables and arbitrary underlying graph structures. In this talk, we will discuss two different parallelizations of the CONCORD algorithm and how we applied communication-avoiding techniques to its main bottleneck, iterative sparse-dense matrix-matrix multiplication, to obtain scalable implementations. We will also present experimental results with real 3D brain fMRI data sets on tens of thousands of cores of a Cray XC30 machine.

Penporn Koanantakool
UC Berkeley
penpornk@eecs.berkeley.edu

Sang-Yun Oh
University of California at Santa Barbara
syoh@pstat.ucsb.edu

Dmitriy Morozov, Aydin Buluc, Leonid Oliker
Lawrence Berkeley National Laboratory
dmorozov@lbl.gov, abuluc@lbl.gov, loliker@lbl.gov

Katherine Yelick
Lawrence Berkeley National Laboratory
University of California at Berkeley
yelick@eecs.berkeley.edu

MS93
Performance of S-step and Pipelined Krylov Methods

We compare the performance of pipelined and s-step variants of a Krylov solver. Our implementations of both s-step and pipelined methods focus on reducing the cost of global all-reduces needed for the orthogonalization. We present performance results on a distributed-memory multicore CPUs to demonstrate the effects of these two methods.

Ichitaro Yamazaki
University of Tennessee, Knoxville
iyamazak@icl.utk.edu

Mark Hoemmen
Sandia National Laboratories
mhoemme@sandia.gov

Jack J. Dongarra
University of Tennessee, Oak Ridge National Laboratory, USA
dongarra@icl.utk.edu

Piotr Luszczek
University of Tennessee
luszczek@icl.utk.edu

MS94
Towards Practically-Efficient Spectral Sparsification of Graphs

Spectral graph sparsification aims to find ultra-sparse subgraphs that can well preserve the eigenvalues and eigenvectors of the original graph Laplacians. The resultant subgraphs can be immediately leveraged for the development of many fast numerical and graph-based algorithms. In this talk, I will first introduce a practically efficient, nearly-linear time spectral graph sparsification method based on a scalable spectral perturbation analysis framework that allows building spectrally-similar yet ultra-sparse subgraphs by recovering small portions of "spectrally critical" off-tree edges to a given spanning tree. Next, I will show how such a spectral sparsification approach can be leveraged for developing much faster algorithms for solving large symmetric diagonally-dominant (SDD) matrices as well as spectral clustering tasks.

Zhuo Feng
Michigan Technological University
zhuofeng@mtu.edu

MS94
On Empirically Evaluating the Performances of Laplacian Solvers

Over the past two decades there has been much theoretical progress on efficient solvers for Symmetric Diagonally Dominant matrices, which are algorithmically equivalent to graph Laplacians. This in turn led to the Laplacian paradigm for designing graph algorithms, which now provide the best runtime guarantees for a wide range of well-studied problems on graphs. This talk will overview recent efforts towards implementations that are an order of magnitude faster than whats currently available, and discuss attempts at benchmarking various solvers and observations made from them. It will discuss in detail ways of benchmarking solvers in ways that isolate the combinatorial, data structural, and numerical aspects, as well as the challenges posed by combinatorial preconditioners to the numerical convergences of iterative methods.

Richard Peng
Georgia Tech
rpeng@cc.gatech.edu

MS94
Asymmetric Multigrid Solver for Sparse Graph Systems of Linear Equations

Finding suitable connectivity measures between variables is one of the key problems in algebraic multigrid. The quality of coarse equations and interpolation scheme as well as the overall complexity of the algorithm directly depend on how well the connectivity between variables is expressed. In

this paper, we propose a simple coarsening mechanism that asymmetrically utilizes connectivity measures between fine and coarse variables in algebraic multigrid often resulting in a faster convergence without significant loss in memory and running time. We demonstrate computational results on graph Laplacian matrices by modifying the Lean AMG solver.

Sloan Nietert, Brian Dean, Ilya Safro
School of Computing
Clemson University
snieter@g.clemson.edu, bcdean@clemdon.edu, isafro@g.clemson.edu

MS94
Scalable Motif-Aware Graph Clustering

In this talk I will present data-driven algorithms for dense subgraph discovery, and community detection respectively. The proposed algorithms leverage graph motifs to attack the large near-clique detection problem, and community detection respectively. In my talk, I will focus on triangles within graphs, but our techniques extend to other motifs as well. The intuition, that has been suggested but not formalized similarly in previous works, is that triangles are a better signature of community than edges. For both problems, we provide theoretical results, we design efficient algorithms, and then show the effectiveness of our methods to multiple applications in machine learning and graph mining. Joint work with Michael Mitzenmacher, and Jakub Pachocki

Charalampos Tsourakakis
CARNEGIE MELLON UNIVERSITY
tsourolampis@gmail.com

MS95
Analysis and Design of Velocity Controllers for Dissipation of Stop-and-Go Traffic Waves

In this talk we describe the design and analysis of three controllers aimed at the dissipation of emergent traffic waves caused by stop-and-go traffic. The controllers take different approaches, with respect to controlling for following distance, following a velocity set point, or adjusting a velocity set point through proportional-integrator control. Each controller uses local information to determine the state of traffic flow, and what the behavior of a controlling vehicle in the flow should be with the objective of dampening traffic waves. The talk will discuss traffic flow instability models used to derive controllers, and the distinct approaches of each controller in order to dampen oscillations. The controllers operate under constraints that are realistic for sensors, computing devices, and actuators that are inexpensive and commercially widespread. The results include regions of operation in which the controllers may be safely engaged, and a summary of the individual controller results from the traffic flow experiment..

Rahul Kumar Bhadani
Electrical and Computer Engineering
University of Arizona, Tucson, AZ 85721-0104, USA
rahulbhadani@email.arizona.edu

MS95
On Well-Posedness and Control of a Moving Bottleneck Model

Recently two models were introduced for moving bottleneck in traffic flow: the first (by Lattanzio, Maurizi and Piccoli) introduces a localized capacity drop in the flow near the bottleneck, while the second (by Delle Monache and Goatin) is based on a pointwise flux constraint. Both models are based on the Lighthill-Whitham-Richards approach consisting of a single conservation laws for the traffic flow. We show continuous dependence results for the two models and estimates on total variation to establish a theory when the moving bottleneck can be controlled. The latter may represent the situation of an autonomous vehicle with controlled speed.

Thibault Liard
Rutgers University - Camden
227 Penn St, Camden, NJ 08102, USA
thibault.liard@rutgers.edu

MS95
Traffic Flow Control and Fuel Consumption Reduction Via Moving Bottlenecks

Moving bottlenecks, such as slow-driving vehicles, are commonly thought of as impediments to efficient traffic flow. Here, we demonstrate that in certain situations, moving bottlenecks—properly controlled—can actually be beneficial for the traffic flow, in that they reduce the overall fuel consumption. As an important practical example, we study a fixed bottleneck (e.g., an accident) that has occurred further downstream. This new possibility of traffic control is particularly attractive with autonomous vehicles, which (a) will have fast access to non-local information, such as incidents and congestion downstream; and (b) can execute driving protocols accurately. Moreover, these controls can be implemented by means of a single control vehicle.

Benjamin Seibold
Temple University
seibold@temple.edu

MS95
Controlling Stop and Go Traffic with a Single Autonomous Vehicle: Experimental Results

This talk explores the problem of controlling human-piloted traffic flows with only a small number of autonomous vehicles. We adopt and refine the experimental setting of Sugiyama et al. (2008), in which 22 vehicles driven by humans on a single lane track are shown to devolve from smooth uniform flow into stop-and-go traffic. In the experiments presented in this work, an intelligently controlled autonomous vehicle replaces a single human-piloted vehicle. A series of experiments in Tucson, Arizona are conducted to measure the influence of the carefully controlled AV on human-piloted vehicles. Trajectory data is extracted from a 360-degree video camera, and the fuel consumption data is logged through each vehicles OBD-II port. The result is a high fidelity and open dataset for further modeling and control development. Our main experimental result indicates that even when the penetration rate of autonomous vehicles is as low as 5%, it is possible to reduce the presence of stop-and-go waves that can appear without the presence of a bottleneck. Our experiments imply that significant improvements in traffic fuel efficiency and safety may be achieved by means of very few mobile actuators in the traffic stream in the near future.

Daniel Work
Civil and Environmental Engineering
University of Illinois at Urbana Champaign, Urbana, IL

61801
dbwork@illinois.edu

MS96

Mechanics of Finite Cracks in Dissimilar Anisotropic Elastic Media Considering Interfacial Elasticity

In this presentation, interfacial crack fields and singularities in bimaterial interfaces (i.e., grain boundaries or dissimilar materials interfaces) are considered through a general formulation for two-dimensional (2-D) anisotropic elasticity while accounting for the interfacial structure by means of a generalized interfacial elasticity paradigm. The interfacial elasticity formulation introduces boundary conditions that are effectively equivalent to those for a weakly bounded interface. This formalism considers the 2-D crack-tip elastic fields using complex variable techniques. While the consideration of the interfacial elasticity does not affect the order of the singularity, it modifies the oscillatory effects associated with problems involving interface cracks. Constructive or destructive "interferences' are directly affected by the interface structure and its elastic response. This general formulation provides an insight on the physical significance and the obvious coupling between the interface structure and the associated mechanical fields in the vicinity of the crack tip. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE–AC04–94AL85000. SAND2017-0798 A

Remi Dingreville
Sandia National Laboratories
USA
rdingre@sandia.gov

PierreAlexandre Juan
Sandia National Laboratories
pjuan@sandia.gov

MS96

On the Role of Surface Effects in the Linear Elastic Fracture Mechanics

In this talk, we present the role of surface effects and crack-tip conditions in the reduction of stress at a crack tip in a theory of linear elastic fracture mechanics. Within the description of the effect of first-order (curvature-independent) surface elasticity, the deformation of linearly elastic isotropic materials containing a crack with sharp edges were examined for both plane and anti-plane deformations. We found that the imposition of boundary conditions at a crack tip is strictly regulated, in each deformation mode, by a distinct maximum number of allowable natural boundary conditions, which subsequently dictate the existence of smooth solutions in the domain of interest. As a result, the first-order theory still predicts unbounded stresses at the crack tips, albeit, in most cases, with a reduced degree of singularity: from the classical strong square-root singularity to the weaker logarithmic singularity. It is worth noting that, the higher-order surface elasticity theory (e.g. Curvature-dependent theory; Steigmann-Ogden surface elasticity) may lead the complete removal of stress singularity at the crack tips, since the higher-order theory can offer the employment of a different set of end-point conditions. In these cases, we obtain a collection of non-standard hypersingular integro-differential

equations for which the existence of admissible, bounded solutions is yet to be decided.

Chun Il Kim
University of Alberta
Canada
cikim@ualberta.ca

Peter Schiavone
Department of Mechanical Engineering
University of Alberta, Edmonton
p.schiavone@ualberta.ca

Ru C-Q
Professor, Department of Mechanical Engineering,
University of Alberta.
c.ru@ualberta.ca

MS96

Regularizing Fracture Boundary Value Problems Via Surface Mechanics

Classical boundary value problems modeling brittle fracture in the setting of the linearized theory of elasticity or viscoelasticity that treat fracture edges as sharp boundaries between perfectly intact material and traction-free fracture surfaces predict stress and strain singularities at fracture edges in contradiction to the infinitesimal strain assumption behind the linearized bulk constitutive equations. This talk surveys recent results on the regularizing effect of modeling fracture surfaces as dividing surfaces endowed with suitably chosen higher gradient stress-strain constitutive behavior.

Jay R. Walton
Department of Mathematics
Texas A&M
jwalton@math.tamu.edu

MS97

Robust and Efficient Multi-Way Spectral Clustering

A common question arising in the study of graphs is how to partition nodes into well-connected clusters. One standard methodology is known as spectral clustering and utilizes an eigenvector embedding as a staring point for clustering the nodes. Given that embedding, we present a new algorithm for spectral clustering based on a column-pivoted QR factorization. Our method is simple to implement, direct, scalable, and requires no initial guess. We also provide theoretical justification for our algorithm and experimentally demonstrate that its performance tracks recent information theoretic bounds for exact recovery in the stochastic block model.

Anil Damle, Victor Minden
Stanford University
asd239@cornell.edu, vminden@stanford.edu

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS97

Multiscale Adaptive Approximations to Data and Functions Concentrated Near Low-Dimensional

Sets

Many data sets in image analysis and signal processing are in a high-dimensional space but exhibit a low-dimensional structure. We are interested in building efficient representations of these data for the purpose of compression and inference. In the setting where a data set in R^D consists of samples from a probability measure concentrated on or near an unknown d-dimensional manifold with d much smaller than D, we consider two sets of problems: low-dimensional geometric approximation to the manifold and regression of a function on the manifold. In the first case we construct multiscale low-dimensional empirical approximations to the manifold and give finite-sample performance guarantees. In the second case we exploit these empirical geometric approximations of the manifold to construct multiscale approximations to the function. We prove finite-sample guarantees showing that we attain the same learning rates as if the function was defined on a Euclidean domain of dimension d. In both cases our approximations can adapt to the regularity of the manifold or the function even when this varies at different scales or locations.

Wenjing Liao, Mauro Maggioni, Stefano Vigogna
Johns Hopkins University
wliao@math.jhu.edu, mauro@math.jhu.edu, svigogna@math.jhu.edu

MS97

A Case for Second Order Algorithms Via Sub-Sampled Newton Methods

Many machine learning, scientific computing and data analysis applications require the solution of optimization problems involving a sum of large number of functions. We first motivate the problem by describing an application from scientific computing, namely PDE-constrained optimization. We then consider a more general problem setting for minimizing a sum of n functions over a convex constraint set. For such problems, algorithms that carefully sub-sample to reduce n can improve the computational efficiency, while maintaining the original convergence properties. For second order methods, we give quantitative convergence results for variants of Newtons methods where the Hessian or the gradient is uniformly sub-sampled. We then show that, given certain assumptions, we can extend our analysis and apply non-uniform sampling which results in modified algorithms exhibiting more robustness and better dependence on problem specific quantities, such as the condition number. We finally present a simple machine learning application demonstrating the properties of our methods.

Fred Roosta, Michael Mahoney
UC Berkeley
farbod@stat.berkeley.edu, mmahoney@stat.berkeley.edu

MS97

Unsupervised Machine Learning - Method and Application

This talk reviews some important unsupervised learning methods that are related to computational linear algebra. These methods have real-world applications like medical data analysis, social media clustering and crime data analysis.

Baichuan Yuan
University of California, Los Angeles
byuan@math.ucla.edu

Andrea L. Bertozzi
UCLA Department of Mathematics
bertozzi@math.ucla.edu

MS98

Waveform Relaxation for Circuit Simulation

Waveform relaxation (WR) methods are based on partitioning large circuits into sub-circuits which then are solved separately over multiple time steps, and the overall solution is obtained by iteration between the sub-circuits. The classical WR approach was developed in the early 1980s for circuit solver applications. However it exhibits slow convergence, especially when long time windows are used. To overcome this issue, optimized WR methods were introduced which are based on optimized transmission conditions that transfer information between the sub-circuits more efficiently than classical WR. These methods are closely related to domain decomposition techniques. We analyze the effect of overlapping sub-circuits in classical and optimized waveform relaxation techniques for RC circuits. We study the influence of overlap on the convergence factor and on the optimization parameter in the transmission conditions. We also show how the optimized parameter behaves close to the limiting case of a particular circuit.

Pratik Kumbhar, Martin J. Gander
University of Geneva
pratik.kumbhar@unige.ch, martin.gander@unige.ch

MS98

Parareal in Fusion Plasma Applications

Long time scale simulations to study the behavior of magnetically confined fusion plasma are arguably one of the 21st centuries HPC Grand Challenges. Studying the physics at the scrape off layer (SOL) in tokamak plasma requires extensive computation. Simulating ELMs (Edge Localized Modes) in this region enhances the complexity of these computations thereby further increasing wallclock times. ELMs lead to release of huge amounts of energy and subject the plasma to sudden, large changes in its dynamics. ELMs are time dependent events and hence, these simulations are particularly challenging when using a time parallelizing algorithm like, Parareal. The Parareal approach involves a predictor-corrector technique typically requiring a coarse and a fine solver. Identification of the optimum coarse solver for a complex problem such as ELMs may often be challenging but not impossible. This work explores various coarse propagators that lead to parareal convergence and also achieve significant reduction in wallclock time thus allowing computational gain. The limitations of each propagator are also studied. The SOLPS (Scrape-Off Layer Plasma Simulator) code package is used for simulating the ELMs. The application uses the Parareal Framework developed at the Oak Ridge National Laboratory as part of the SWIM IPS project.

Debasmita Samaddar
CCFE
UK Atomic Energy Authority
Debasmita.Samaddar@ukaea.uk

David Coster
Max-Planck-Institut für Plasmaphysik, Germany
david.coster@ipp.mpg.de

Xavier Bonnin

ITER Organization, France
xavier.bonnin@iter.org

Wael R. Elwasif, Lee A. Berry
ORNL, USA
elwasifwr@ornl.gov, leeaberry223@gmail.com

Donald B. Batchelor
Oak Ridge National Laboratory
batchelordb@ornl.gov

MS98

Asymptotic Convergence of PFASST for Linear Problems

For time-dependent PDEs, parallel-in-time integration using the "parallel full approximation scheme in space and time" (PFASST) is a promising way to accelerate existing space-parallel approaches beyond their scaling limits. Inspired by the classical Parareal method and non-linear multigrid ideas, PFASST allows to integrate multiple time-steps simultaneously using "multi-level spectral deferred corrections" with different coarsening strategies in space and time. In numerous studies, this approach has been successfully coupled to space-parallel solvers which use finite differences, spectral methods or even particles for discretization in space. While many use cases and benchmarks exist, a solid and reliable mathematical foundation is still missing. In this talk, we use the recent formulation of PFASST as a multigrid to analyze the asymptotic convergence behavior for small time-step sizes as well as for large numbers of degrees-of-freedom. We derive bounds for the spectral radius of the two-level iteration matrix and compare these findings with experimental results.

Robert Speck
Juelich Supercomputing Centre
Forschungszentrum Juelich GmbH
r.speck@fz-juelich.de

Dieter Moser
Juelich Supercomputing Centre
Forschungszentrum Juelich
d.moser@fz-juelich.de

Matthias Bolten
University of Wuppertal
Germany
bolten@math.uni-wuppertal.de

MS99

PCA and Curvature: Numerical Examples on Spaces of Landmarks

Principal Component Analysis (PCA) is a widely used tool for analyzing high-dimensional data. In many shape applications data lies on a manifold M, and PCA is applied through the linearization of the points on the manifold via the tangent space representation $T_\mu M$ at the Karcher mean μ. This linearization fails to account for curvature of the underlying manifold. In this talk I will demonstrate an approach to take into account curvature and to better capture variance of the data. Some numerical experiments will be demonstrated.

Sergey Kushnarev
Singapore University of Technology and Design
sergey_kushnarev@sutd.edu.sg

MS99

Retinal Morphometrics in Aging and Glaucoma using the Fshape Framework

Fshape is a novel approach for quantitative shape variability analysis using surface geometry with functional measures for registration across anatomical shapes. We have applied the fshape framework to characterize the effects of aging and glaucoma in the retinal nerve fiber layer (RNFL) and choroid. We generated group-wise mean retinal nerve fiber layer and choroidal surface templates with the respective layer thicknesses. We then generated fshapes mapping of all observations to the mean templates and showed the difference by age and by glaucoma in each layers. We then compared these findings with a more conventional sector-based analysis for comparison. The fshape results visualized the detailed spatial patterns of the differences between the age-matched normal and glaucomatous retinal nerve fiber layers, with the latter most significantly thinner in the inferior region close to Bruchs membrane opening. Between the young and older normal cases, choroid was shown to be significantly thinner in the older subjects across all regions, but particularly in the nasal and inferior regions. The results demonstrate a comprehensive and detailed analysis of retinal morphometrics using the fshape framework and compared to the existing state-of-art sectoral averaging approaches, fshapes extends the ability to now observe point-wise changes that have the potential to reveal localized small changes that may be due to disease such as glaucoma earlier than currently possible.

Sieun Lee
Simon Fraser University
leeau@sfu.ca

MS99

A Convenient Numerical Scheme to Compute the Parallel Transport Along Geodesics

Parallel transport is interesting in the context of shape analysis because it brings longitudinal evolutions into a common frame of reference in an isometric way. The main methods to compute the parallel transport require either to compute Riemannian logarithms, such as Schild's ladder, or to compute the Christoffel symbols. In both cases, these computations are often intractable or very expensive. From an identity between parallel transport and jacobi fields, we propose a numerical scheme to approximate the parallel transport along a geodesic. We prove a convergence rate equivalent to Schild's ladder, while controlling the number of computational steps. We then illustrate the algorithm with actual examples.

Maxime Louis
Brain and Spine Institute (ICM), Paris
maxime.louis.x2012@gmail.com

MS99

Frequency Diffeomorphisms for Efficient Image Registration and Bayesian Statistical Shape Analysis

Investigating clinical hypotheses of diseases and their potential therapeutic implications based on large medical image collections is an important research area in medical imaging. Medical images provide an insight about anatom-

ical shape changes caused by diseases; hence is critical to disease diagnosis and treatment planning. Characterization of the anatomical shape changes poses computational and statistical challenges due to the high-dimensional and nonlinear nature of the data, as well as a vast number of unknown model parameters. In this talk, I will present efficient, robust, and reliable methods to address these problems. My approach entails (i) developing a low-dimensional shape descriptor to represent anatomical changes in large-scale image data sets, and (ii) novel Bayesian machine learning methods for analyzing the intrinsic variability of high-dimensional manifold-valued data with automatic dimensionality reduction and parameter estimation. The potential practical applications of this work beyond medical imaging include machine learning, computer vision, and computer graphics.

Miaomiao Zhang
Massachusetts Institute of Technology
miao86@mit.edu

MS100

Numerical Methods for Kinetic Equations in the Anomalous Diffusion Limit: Critical Exponent for a Heavy-Tailed Equilibrium

We consider a kinetic equation for which the equilibrium is a heavy-tailed function. The scaling of the kinetic equation is chosen depending on the decrease of the tail, and the asymptotic regime is either a diffusion equation of a fractional diffusion equation. We consider here a critical case, for which the asymptotic equation is a diffusion equation, but with an anomalous time scale. We will explain the asymptotic behavior of the kinetic equation, since the convergence towards the limit equation is very slow. We will then present asymptotic schemes for this case, which are designed to deal with this logarithmic convergence. Eventually, numerical tests are presented.

Helene Hivert
Unité de Mathématiques Pures et Appliquées
helene.hivert@ens-lyon.fr

MS100

Schwartz Duality for the Spectral Collocation Approximation to the Fractional Advection Diffusion Equation with Singular Source

Spectral methods provide accurate approximations to fractional PDEs when the solution is smooth. However, if the solution is not smooth the spectral approximation is highly oscillatory. In this talk, we present a high order numerical method using the Chebyshev spectral collocation method for the fractional diffusion type equation when highly localized source term is existent. The presented methodology is to construct a consistent spectral algorithm to the singularity based on the Schwartz duality. Numerical examples will be presented.

He Yang
Ohio State University
yang.1671@osu.edu

Jingyang Guo, Jae-Hun Jung
SUNY at Buffalo

jguo4@buffalo.edu, jaehun@buffalo.edu

MS100

Numerical Methods for Kinetic Equations in the Anomalous Diffusion Limit: Heavy-Tail Equilibria and Singular Collision Frequencies

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Mohammed Lemou
IRMAR, University of Rennes 1
mohammed.lemou@univ-rennes1.fr

MS100

Asymptotic Preserving Schemes for Anisotropic Transport Equation with Fractional Diffusion Limit

For linear transport equation with diffusive scaling, classical diffusion may fail when the diffusion matrix becomes unbounded, which can be attributed to two reasons. One comes from the heavy tail equilibrium and the other is due to the degenerate collision frequency. In this talk we present asymptotic preserving schemes for both cases. The former one relies on a micro-macro decomposition along with a body-tail decomposition, and the latter one takes a special care in integrating a singular function.

Li Wang
State University of New York, Buffalo, USA
lwang46@buffalo.edu

MS101
Ensemble Simulation Models and Algorithms

Repeated computations of flow equations with varying parameters are commonly seen in many engineering and geophysical applications as an effort to deal with inherent uncertainties. These computations are generally treated as independent tasks. While parallel computing can save computational time in this setting, no savings are realized in terms of total computational cost. In this talk, we will describe a new way to perform multiple simulations efficiently, in terms of both storage and computational cost. The proposed algorithm computes all realizations at one pass by adopting an ensemble time-stepping scheme, which results in the same coefficient matrix for all realizations. This reduces the problem of solving multiple linear systems to solving one linear system with multiple right-hand sides, for which many efficient methods, e.g., block CG, block QMR, block GMRES, can be applied to significantly save the computation cost.

Nan Jiang
Missouri University of Science and Technology
jiangn@mst.edu

MS101
Artificial Compression Methods

Artificial compression methods are the fastest way to solve the incompressible Navier-Stokes equations. They are also among the least used when a reliable answer is required due to stability issues, issues with parasitic, fast acoustic waves and nonphysical predictions. This talk will present a new AC algorithm which is provable stable, damps nonphysical acoustics even at higher Reynolds numbers and is easily implemented so as to preserve physical fidelity of the low Mach number approximation. This is joint work with

Victor Decaria, Joe Fiordelino, Michael McLaughlin and Haiyun Zhao. Given a fast and memory efficient algorithm, the next step, currently under study, is to extend it to compute an ensemble of solutions.

William Layton
University of Pittsburgh
wjl+@pitt.edu

MS101

Numerical Analysis and Computations of Sensitivities in Fluid Flow Problems

We present a computational study of the sensitivity of the Navier Stokes regularization models with respect to the filter diameter. The sensitivity of the models is evaluated in 2-D as well as 3-D problems. In both cases, a wide range of filter diameter values and Reynolds numbers are considered. These experiments were computed by solving the sensitivity equations technique for the models.

Monika Neda
University of Nevada Las Vegas
monika.neda@unlv.edu

MS101

New Results for the EMAC Scheme for Incompresssible Navier-Stokes Simulation

We first review the recently proposed EMAC scheme, which is based on a new formulation of the NSE that conserves each of discrete energy, momentum, angular momentum, helicity and vorticity, even when the divergence constraint is not exactly satisfied (e.g. when commonly used mixed finite elements like Taylor-Hood are used). We then discuss properties of the scheme when different linearizations are applied, and give results for several benchmark problems which illustrate how using schemes with more accurate discrete physics leads to better overall accuracy.

Leo Rebholz
Clemson University
Department of Mathematical Sciences
rebholz@clemson.edu

PP1

A Review of the Poincare-Bendixson Theorem and Its Extensions

The Poincare-Bendixson theorem is a powerful tool in dynamical systems. It gives us a way to determine the existence of periodic solutions on planar surfaces. It also describes the structure of limit sets in such systems and rules out chaos in the two-dimensional space. To apply the Poincare-Bendixson theorem, the usual method is to construct a trapping region R which is a bounded region with a single repelling equilibrium or an annular region with no equilibrium. Then every trajectories that starts in R cannot leave it, thus proving the existence of a periodic solution.
In this poster we present a review of the classic theorem and some modern results associated with it, including extensions of the theorem to higher dimensions.

Nazila Akhavan Kharazian, Felicia Magpantay
University of Manitoba
akhavann.myumanitoba.ca,   felicia.magpantay@umanitoba.ca

PP1

A Comparison of Existing Measles Models

With improvements in computational power, more and more mechanistic models have been formulated to explain physical and biological phenomena. In this poster we assess the strengths and weaknesses of different well-known models of pre-vaccine era measles dynamics. We compare them with respect to their fit to data and how they perform when extended to the vaccine era dynamics. The models studied include the standard SEIR model with forcing, the TSIR model [Bjrnstad et al, Dynamics of Measles Epidemics : Estimating Scaling of Transmission Rates Using a Time Series SIR Model].

Clifford Allotey, Felicia Magpantay
University of Manitoba
cliffora@myumanitoba.ca,   felicia.magpantay@umanitoba.ca

PP1

Nonlinear Phenomena in a Piecewise Linear Model of Airflow in Birds Lungs

Avian lungs are remarkably different from mammalian lungs in that air flows unidirectionally through rigid tubes where gas exchange takes place. This unidirectional flow occurs across a wide range of breathing frequencies, amplitudes, and specific species anatomies. It has been hypothesized that the unidirectional flow is due to aerodynamic valving, resulting from the complex anatomical structure of the avian lung and the fluid dynamics involved. To test this hypothesis, we have constructed a novel mathematical model that, unlike previous models, can produce unidirectional flow which is robust to changes in model parameters, breathing frequency and breathing amplitude. The model consists of two piecewise linear ordinary differential equations with lumped parameters and discontinuous, flow-dependent resistances that mimic the experimental observations. The model provides several new physiological insights into the lung mechanics of birds and also serves as a new example of a piecewise linear model that exhibits nonlinear phenomena (such as symmetry breaking).

Alona Ben-Tal
Massey University
Institute of Information & Mathematical Sciences
a.ben-tal@massey.ac.nz

Emily Harvey
m.e market economics
emily@me.co.nz

PP1

Bootstrapping and Cross-Validating Generalized Pls Regressions Using Gpu

Processes based on the so-called Partial Least Squares (PLS) regression, which recently gained much attention in the analysis of high-dimensional genomic datasets, were recently developed to perform variables selection. Most of these processes rely on some tuning parameters that are usually determined by Cross-Validation (CV), which raises important stability issues. We have developed a new dynamic bootstrap based PLS process for significant predictors selection, suitable for both PLS regression and its

extension to Generalized Linear (GPLS) regression frameworks. Since it has a very computational cost, we developed a GPU based R package to speed up our existing package plsRglm. The aim of the plsRglm package is to deal with complete and incomplete datasets through several new techniques or, at least, some which were not yet implemented in R. Indeed, not only does it make available the extension of the PLS regression to the generalized linear regression models, but also bootstrap techniques, leave one-out and repeated k-fold cross-validation. In addition, graphical displays help the user to assess the significance of the predictors when using bootstrap techniques. Biplots can be used to delve into the relationship between individuals and variables.

Frederic Bertrand
Universite de Strasbourg
fbertran@math.unistra.fr

Myriam Maumy
Universite de Strasbourg
IRMA
mmaumy@math.unistra.fr

PP1

The Reduced Collocation Method for Nonlinear Steady-State PDEs

Reduced basis methods are a class of numerical methods developed for settings which require a large number of solutions to a parameterized problem. In this work, we consider settings which require many queries to a numerical solver for a parameterized steady-state partial differential equation. We adapt an existing method for linear steady-state problems, the reduced collocation method, to the nonlinear case.

Chris Bresten, Yanlai Chen
University of Massachusetts Dartmouth
cbresten@umassd.edu, ychen5@umassd.edu

PP1

Modeling the Effect of Calcium Coupling on Sperm Motility

Changes in calcium concentration along the sperm flagellum regulates sperm motility and hyperactivation, characterized by an increased flagellar bend amplitude and beat asymmetry, enabling the sperm to reach and to penetrate the oocyte. However, the exact mechanisms of calcium signaling are yet unknown and under investigation. We develop a fluid-structure interaction model that couples the three-dimensional motion of the flagellum in a highly viscous Newtonian fluid with the calcium dynamics in the flagellum. The flagellum is modeled as a Kirchhoff-rod: an elastic rod with intrinsic curvature and twist. The calcium dynamics are represented as a one-dimensional reaction-diffusion model on the moving flagellum. The two models are coupled assuming that the sperm flagellum preferred curvature depends on the evolving calcium concentration in time. To investigate the effect of calcium on sperm motility, we compare model results of flagellar bend amplitude and swimming speed for different phenomenological functions representing the dependence of curvature on the calcium concentration.

Lucia Carichino, Sarah D. Olson
Worcester Polytechnic Institute

lcarichino@wpi.edu, sdolson@wpi.edu

PP1

Mathematical Modeling of Tissue Engineered Articular Cartilage

Articular cartilage has a complex structure composed of a dense extracellular matrix (ECM), which includes fluid, a collagen network, and other proteins. Distributed in the matrix there are chondrocytes (cells) that synthesize the building blocks of the ECM. Pathologies such as osteoarthritis, injuries and normal wear and tear can cause the erosion and damage of articular cartilage. Tissue engineering represents a promising path towards the treatment of damaged cartilage. In this work, a hybrid mathematical model is used to investigate the phenomena of cartilage growth in a tissue-engineered construct to elucidate and clarify the influence of different biological factors and conditions involved in the process. This hybrid model couples a discrete modeling approach for the chondrocytes, with a continuous approach for the remaining components of the matrix, modeled via a time dependent diffusion-reaction equation. We investigate the influence of different scaffold properties and cell seeding on the synthesis of new ECM. The insight provided by the model will be used to elucidate some of the outcomes of laboratory experiments involving tissue-engineered articular cartilage.

Simone Cassani, Sarah D. Olson
Worcester Polytechnic Institute
scassani@wpi.edu, sdolson@wpi.edu

PP1

A Posteriori Analysis of the Poisson-Boltzmann Equation

The Poisson-Boltzmann equation (PBE) models the electrostatic interactions of charged bodies such as molecules and proteins in an electrolyte solvent. The PBE is a challenging equation to solve numerically due to the presence of singularities, discontinuous coefficients and boundary conditions. Hence, there is often large error in numerical solutions that needs to be quantified. In this work, we use adjoint based a posteriori analysis to accurately quantify the error in an important quantity of interest, the solvation free energy. We identify various sources of error and propose novel refinement strategies based on a posteriori error estimates.

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

PP1

A Three-Sensor Assignment Method for Multiple Target Tracking

Multiple sensors reduce uncertainty when tracking targets using noisy position measurements. However, measurements from different sensors must be matched. In the case of two 2-dimensional and one 3-dimensional sensors, we develop a statistical model and solve a combinatorial optimization problem to determine the pair of permutations that provides the best match. By formulating the problem in five rather than four-dimensional space, we enforce an additional constraint which can rule out suboptimal matches.

Cesar Contreras, John Langford, Larry Ammann, John

Zweck
University of Texas at Dallas
cxc145430@utdallas.edu, jxl128231@utdallas.edu, ammann@utdallas.edu, jwz120030@utdallas.edu

PP1

Corrupted Blood: A Mathematical Analysis

In 2005, a virtual plague called Corrupted Blood (CB) swept through Blizzard's MMORPG World of Warcraft, leaving thousands of players unable to play. With a 100% transfer rate and a predictable transmission pattern, the spread of infection can be modeled as a function of time. Using a MatLab simulation and differential equations for data analysis, we found that the spread of CB (and potentially other diseases) can be modeled as a transformation of the Sigmoid function.

Kyle Cook, Anthanasios Gentimis
Florida Polytechnic University
kcook2499@flpoly.org, agentimis@flpoly.org

PP1

Modeling and Simulation of Phytoplankton Blooms in the Ocean

Phytoplankton are the base of the marine food web. They are also responsible for almost half of the oxygen we breathe as they remove carbon dioxide from the atmosphere. A macroscale plankton ecology model is constructed consisting of coupled, nonlinear reaction-diffusion equations with spatially and temporally changing coefficients. A variation of an NPZ model, this model simulates biological interactions between nutrients, phytoplankton and zooplankton. It also incorporates seasonally varying, physical driving forces that affect phytoplankton growth: solar radiation and depth of the ocean's upper mixed layer. The model is analyzed using seasonal oceanic data with the goal of understanding seasonal changes in plankton biomass. This can be helpful to understand the ecological structure of plankton communities and the timing of seasonal phytoplankton blooms, which are debated topics in oceanography.

Seth Cowall
University of Delaware
sethcowall@comcast.net

L. Pamela Cook
University of Delaware
Department of Mathematical Sciences
cook@udel.edu

Matthew J. Oliver
University of Delaware
School of Marine Science and Policy
moliver@udel.edu

PP1

A New Algorithm for Community Detection in Large Social Networks

Networks provide a useful representation for the investigation of complex systems, and makes it possible to examine the intermediate-scale structure of such systems. Consequently, networks have attracted considerable attention in sociology, biology, computer science, and many other disciplines. The majority of intermediate-scale structure investigations have focused on community structure, where one decomposes the network into cohesive groups of nodes referred to as communities, which have a higher density of connections within than between them. With the rise of social media (e.g Facebook and Twitter), algorithms for community detection in large social networks have become increasingly important. In this work we propose a new algorithm for community detection. The algorithm proceeds by alternating three simple routines in an iterative fashion: diffusion, thresholding, and random sampling. We use our algorithm to detect communities in a large social network of 4.8 million users known as the LiveJournal Network. We compare the performance of our algorithm with a state of the art algorithm developed by Facebook. We also conduct a thorough study of the mathematical properties of the proposed algorithm. We show that the algorithm monotonically increases some quality function describing how good is the partition of the network.

Natalia Y. Dibbern
Student
ndibbern@lion.lmu.edu

Thomas Laurent
Loyola Marymount University
thomas.laurent@lmu.edu

PP1

Open-Source Python Package for Easy and Flexible Shape Optimization and Analysis

Many problems in science and engineering are expressed as shape optimization problems, in which the variable is a shape such as a curve in 2d or a surface in 3d. Examples are optimization of the shape of an airplane wing, and delineation of boundaries of biological structures in medical scans. We typically express such problems as energies with data (or target) mismatch and geometric regularization components, to be minimized algorithmically to attain the optimal shape. To solve such problems, we have implemented a suite comprising various building blocks of such problems and algorithms to perform the minimization, including geometric regularization, statistical shape priors, adaptive geometric discretization, and fast Newton-type minimization schemes. Moreover, we have developed crucial shape analysis algorithms for statistical analysis and evaluation of the shapes computed, based on elastic shape distance framework. Our main applications are image and data analysis problems, but the infrastructure is quite general, and can be used for problems in other fields as well. All our algorithms are implemented in Python, leveraging on the NumPy/SciPy ecosystem, making them as easy to use as Matlab, also compatible with existing Python tools. Our algorithms will be freely available as an open source package for the research community at: http://scikit-shape.org

Gunay Dogan
Theiss Research, NIST
gunay.dogan@nist.gov

PP1

Numerical Study of Flow and Transport in EOR Processes

A macroscale model for multiphase, multicomponent flows through porous media and a hybrid numerical method are presented [1]. This model relies on a new global pressure formulation that has been defined in the context of differ-

ent chemical enhanced oil recovery processes like polymer flooding and surfactant-polymer flooding. The model comprises of a coupled, highly nonlinear system of governing equations which is solved by a hybrid numerical method that combines a non-traditional finite element method, capable of efficiently resolving discontinuities, with a high-order characteristics-based finite difference method. Simulation studies are presented to compare with available approximate models and also to investigate the effect of relevant parameters like multiscale heterogeneity and mobility ratios on the flow pattern. These studies can help in the design of optimal injection policies for chemical EOR as well as in understanding the development and growth of fingering patterns. Simulation results are also presented with different injection policies and the relative performance of these schemes are compared by calculating recovery efficiency. This work has been supported by QNRF NPRP grant 08-777-1-141 and NSF grant DMS-1522782.

[1] P. Daripa, S. Dutta, *Modeling and simulation of surfactant-polymer flooding using a new hybrid method*, Journal of Computational Physics, **335**, 249–282 (2017).

Sourav Dutta
Texas A&M University
sdutta@math.tamu.edu

Prabir Daripa
Department of Mathematics
Texas A&M University
daripa@math.tamu.edu

PP1

Parameter Identifiability and Sensitivity in a Wound Healing Mathematical Model

Since the medical treatment of diabetic foot ulcers remains a challenge for clinicians, a quantitative approach using de-identified patient data and mathematical modeling can help researchers understand the physiology of the wounds. The goal of this project is to utilize individual patient data to identify key parameters, through the use of nonlinear mixed effects modeling, Latin hypercube sampling (LHS), partial rank correlation coefficients (PRCC), and delayed rejection adaptive metropolis (DRAM), in the healing process in order to improve patient care and diagnosis. In this work, we plan to use nonlinear mixed effects modeling to attribute wound healing variability to either fixed effects, parameters that are more likely to remain constant for all patients, or random effects, parameters that vary from patient to patient. The identified random effects should then be taken into special consideration when treating patients with chronic wounds, especially diabetic foot ulcers. We will also use LHS, a stratified sampling method, in conjunction with PRCC, computed from a multivariable regression analysis, to identify the sensitivities of parameters. A Bayesian approach using DRAM, a MATLAB implementation of a Metropolis-Hastings algorithm, will also be used to estimate and analyze parameters. Using DRAM can help with parameter estimation since the available data is sparse and can help find parameter identifiability issues.

Rachel N. French, Rachel Turner, Jacob Menix
Western Kentucky University
rachel.french786@topper.wku.edu,
rachel.turner937@topper.wku.edu,   ja-
cob.menix841@topper.wku.edu

PP1

A Mathematical Model of Microwave Heating a Dielectric Layer for Channel Flow Energy Collection

The use of heat exchangers to harness electromagnetic energy has great potential in transmitting and collecting beamed energy through space. We consider a simple three-layer laminate model in which a middle layer characterized by a temperature-dependent loss factor is surrounded by two lossless dielectric fluid layers. When the fluid is still and plane waves are symmetrically applied with normal incidence to the laminate, a Bragg interference effect occurs when the loss factor in the middle layer is held fixed. In ceramic materials the loss factor depends on temperature, and we find a new stable steady-state solution corresponding to these resonance conditions, whose equilibrium temperature is significantly elevated but saturates before the onset of thermal runaway. Using a lubrication approximation for momentum and energy conservation when fluid motion is imposed, we examine steady-state energy profiles and determine how the fluid motion affects these new solutions. Impacts to improving energy harnessing are discussed.

Joseph M. Gaone
Worcester Polytechnic Institute
Department of Mathematical Sciences
jmgaone@wpi.edu

Burt S. Tilley
Worcester Polytechnic Institute
Mathematical Sciences Department
tilley@wpi.edu

Vadim Yakovlev
Worcester Polytechnic Institute
vadim@wpi.edu

PP1

Assessing the Growth of Ung Family: A Logistic Approach

With the consolidation of campuses and becoming a four year institution, it was observed that the University of North Georgia campus population is growing at an alarming rate. In this work we established a mathematical model that closely depicts the UNG population in contrast to the varying differential parameters. we first tested it against a constant predation rate, namely growing tuition. We found non linear implicit solutions to the system of ODE's and approximated the solutions using numerical methods.

Elizabeth M. Gilman
University O North Georgia
emgilm8571@ung.edu

Bikash Das
University of North Georgia
bikash.ds@ung.edu

PP1

Geometry of 3D Environments and Sum of Squares Polynomials

Motivated by applications in robotics and computer vision, we study problems related to spatial reasoning of a 3D envi-

ronment using sublevel sets of polynomials. These include: tightly containing a cloud of points (e.g., representing an obstacle) with convex or nearly-convex basic semialgebraic sets, computation of Euclidean distances between two such sets, separation of two convex basic semalgebraic sets that overlap, and tight containment of the union of several basic semialgebraic sets with a single convex one. We use algebraic techniques from sum of squares optimization that reduce all these tasks to semidefinite programs of small size and present numerical experiments in realistic scenarios.

Georgina Hall, Amir Ali Ahmadi, Amir Ali Ahmadi
Princeton University
gh4@princeton.edu, a_a_a@princeton.edu,
a_a_a@princeton.edu

PP1
Discovering Brain Networks Using Tensor Decompositions

Tensors and their decompositions are gaining popularity in a variety of fields as a means to find underlying patterns in large and complex data sets. In this work we use the CANDECOMP/PARAFAC or CP Decomposition to discover and differentiate brain networks in fMRI data gathered from human subjects exhibiting varying psychological disorders, including Major Depressive (MDD), Social Anxiety (SAD), and Comorbidity (COMO). Existing literature has demonstrated the use of CP Decomposition in finding and differentiating brain networks associated with tasks such as word associations[2]. Here we again show that the CP Decomposition can be used to find task associated patterns and brain activity. However, we also 1) demonstrate results in finding correlated brain networks associated with positive and negative emotional states and 2) use a technique called Coupled Matrix Tensor Factorization (CMTF)[1] to find differentiating components among subject groups performing the same tasks. On the computational side we have implemented high performance code for the CMTF algorithm using two different techniques. We compare the Alternating Least Squares (ALS) method, which is the standard algorithm for CP without matrix coupling, and the All-at-Once Optimization approach which has been shown to have certain advantages over ALS for CMTF [1].

Koby B. Hayashi, Grey Ballard, Michael Tobia
Wake Forest University
hayakb13@wfu.edu, ballard@wfu.edu, tobiamj@wfu.edu

PP1
Seismogram Classification Using Learned Convolutional-Filter Dictionaries

Seismic inversion is the process of using seismic data to estimate the geophysical properties of the earth. The inversion process requires that practitioners choose a specific model of the subsurface, based on physical intuition. These models can range from simple one-dimensional, homogeneous, stratified subsurface layers to more complicated elasticity models including anisotropy and heterogeneity. However, given a set of seismic measurements there is no agreed upon methodology to determine, *a priori*, the necessary model complexity required to accurately represent the subsurface. To advance a solution to this problem we have developed a classification algorithm for seismic-inversion model selection. Our algorithm is based on learning a dictionary of convolutional filters using synthetically generated seismograms from a discrete set of possible subsurface models.

For each possible subsurface model a filter dictionary, capable of sparsely representing seismograms generated from that model, is learned. A given seismogram is then classified as being generated from the subsurface model whose filter dictionary yields the most accurate, and sparse, reconstruction. We demonstrate our algorithm on a synthetic data set consisting of eight distinct subsurface model classes. Through a series of cross-validation experiments, we show that our algorithm can accurately identify the presence, or absence, of some subsurface features.

Kyle S. Hickmann
Los Alamos National Laboratory
hickmank@lanl.gov

Gowri Srinivasan
T-5, Theoretical Division, Los Alamos National
Laboratory
gowri@lanl.gov

PP1
A Tensor Field Mumford-Shah Segmentation of Neural Pathways in Diffusion Weighted MRI Images

Owing to the structural features of the brain, water diffusion is facilitated along the direction of neural pathways, and hindered in the transverse direction against cell walls. Diffusion MRI images, measure the rates of diffusion of water molecules, in various directions, at each spatial point of the brain; assuming a Gaussian distribution of diffusion, these measurements can be summarized by 3x3 diffusion tensor at each point, which gives diffusion magnitude and orientation information. This information is valuable in mapping neural pathways in the brain. In this work, we propose a level set variational approach to segment the neural pathways, similar to Mumford-Shah segmentation, but adapted to tensor field information we have. The approximating tensor field is set to be piecewise constant in the shape and piecewise smooth in the orientation. We test our approach on synthetic and real diffusion weighted MRI images. We present some of the challenges of optimizing the nonlinear energy functional of our model.

Bebart Janbek
Department of Mathematics
Simon Fraser University
bjanbek@sfu.ca

Brian Booth, Ghassan Hamarneh
Simon Fraser University
Medical image analysis lab
bgb2@sfu.ca, hamarneh@sfu.ca

PP1
Yield to the Resistance: The Impact of Nematode Resistant Varieties on Alfalfa Yield

Alfalfa is a major cash crop in the western United States, where it is common to find fields that are infested with the alfalfa stem nematode (Ditylenchus dipsaci). With no nematicides available to control nematode spread, growers can use nematode resistant varieties of alfalfa to manage nematode populations in a field. I present a deterministic, discrete-time, host-parasite model that describes the spread of alfalfa stem nematodes on resistant hosts. Numerical results obtained from simulations with the model are used to compare how varying levels of resistance can affect harvest yield. Results show that switching from a

low resistant rating to a high resistant rating can approximately double the yield over the lifetime of the alfalfa crop.

Scott G. Jordan, Luis Gordillo
Utah State University
scottjordan@aggiemail.usu.edu, luis.gordillo@usu.edu

PP1
Identifying Optimal Sampling Distributions for Individual Patients with Diabetic Foot Ulcers

In this work, we utilized a previously developed mathematical model describing the interactions among matrix metalloproteinases, their inhibitors, extracellular matrix, and fibroblasts (Krishna et al., 2015). The model was modified and curve-fitted to individual patient data from Muller et al. (2008), while model parameters were estimated using ordinary least-squares. The individual parameter measurements were then used in a Fisher information matrix (FIM) to calculate local sensitivity values and time evolution of the sensitivities. We then used the FIM to identify the optimal final times for each patient. This information was included with the standard-error optimal-design algorithm to determine optimal sampling distributions for each patient.

Nigar Karimli, Ayush Prasad, Richard Schugart
Western Kentucky University
nigar.karimli042@topper.wku.edu,
ayush.prasad520@topper.wku.edu,
richard.schugart@wku.edu

PP1
Sufficient Conditions for Existence of Stationary Distributions of Stochastic Reaction Networks and Mixing Times

Reaction networks are graphical configurations that can be used to describe biological interaction networks. If the abundances of the constituent species of the system are low, we can model the system as a continuous time Markov jump process. In this work, we will focus on which conditions of the graph imply existence of stationary distributions for the associated Markov process. We also present results related to their mixing times, which give the time required for the distribution of the Markov process to get close to the stationary distribution.

Jinsu Kim
University of Wisconsin-Madison
jkim522@wisc.edu

David F. Anderson
Department of Mathematics
University of Wisconsin Madison
anderson@math.wisc.edu

PP1
Matrices, Moments, Quadrature and Pdes

Krylov subspace spectral (KSS) methods are high-order accurate, explicit time-stepping methods with stability characteristic of implicit methods. This "best-of-both-worlds' compromise is achieved by computing each Fourier coefficient of the solution using an individualized approximation, based on techniques from "matrices, moments and quadrature' due to Golub and Meurant for computing bilinear

forms involving matrix functions. This poster will present an overview of their derivation and essential properties, and also highlight ongoing projects aimed at enhancing their performance and applicability.

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

PP1
The Influence of a Lipid Reservoir on the Tear Film Dynamics

We present a mathematical model to study the influence of a lipid reservoir, seen experimentally, at the lid margins on the formation and relaxation of the tear film during a partial blink. Applying the lubrication limit, we derive two coupled non-linear partial differential equations characterizing the evolution of the aqueous tear fluid and the covering insoluble lipid concentration. Differently, from prior works, we explore a new set of boundary conditions enforcing desired lipid concentration dynamics at the lid margins. By approximating the equations, both numerically and analytically, we find the lipid-focused boundary conditions create interesting dynamics near the lid margins and therefore significantly impact tear film thinning rates. Specifically, during relaxation, the presence of the lipid reservoir slows down tear film thinning, whereas, during the opening phase of the eye, it accelerates thinning. More importantly, this work points out the limitation of the lubrication theory in capturing the dynamics of the tear film near the lid margins.

Kara L. Maki
School of Mathematical Sciences
Rochester Institute of Technology
kmaki@rit.edu

Gregory Barron
Rochester Institute of Technology
gab1232@mail.rit.edu

Richard Braun
University of Delaware
rjbraun@udel.edu

PP1
Heat Transfer and Flow of a Non-Linear Fluid

Flow of mixtures composed of solid particles of various shapes and sizes dispersed in a fluid occurs in many industrial processes as well as in nature. Examples of such complex fluid mixtures are coal slurries and drilling fluids. Drilling fluids are generally water-based or oil/polymer-based. In the formulation of either the water-based or the oil-based drilling fluids several additives are added to maintain proper rheological properties. These additives, and the fact that drilling fluids are composed of mud, pieces of rocks, water, oil, bubble, etc., make the drilling fluid behave as complex non-Newtonian fluids. In this presentation we study the effects of viscous dissipation in the Couette flow and heat transfer in a drilling fluid, and explore the effects of concentration and the shear-rate and temperature-dependent viscosity, along with a variable thermal conductivity. A brief discussion on the constitutive relations for the stress tensor, the diffusive particle flux vector, and the heat flux vector is presented. The one-dimensional forms of the governing equations are solved numerically and the re-

sults are presented through a parametric study by varying the dimensionless numbers.

Mehrdad Massoudi
National Energy Technology Laboratory
U. S. Department of Energy
MASSOUDI@NETL.DOE.GOV

Wei-Tao Wu
Biomedical Engineering
Carnegie Mellon University
weitaow@andrew.cmu.edu

PP1
Interactive Visualization for the Reading and the Pattern Identification of the Electrocardiogram Using R Shiny

The electrocardiogram (ECG) represents a signal of the electrical activity from heart, this is a non-invasive means to observe the behavior of the heart [T. Garcia, 12-lead ECG: The art of interpretation]. Thanks to the technological advances of the 21st century, there are portable medical devices for recording and storing massive data volumes of ECG, opening the possibility to investigate a new process that optimally uses the information contained in the ECG [P. De Chazal, Automatic classification of heart-beats]. It examines mathematical and statistical methods, supported by digital signal processing, and multivariate tools such as the Andrews curve, which contribute for easy data manipulation, visualization and pattern extraction; for these are evaluated its impact on the medical area dedicated to the diagnosis of cardiovascular diseases. With this study, an interactive application was made using the Rstudio IDE and its shiny library, which selects a previously filtered segment of about 50 cycles of one ECG channel (channel II) allowing a simple interaction between the user and the products such as: the location of the R spike, the visualization and detection of the P and T waves for each of their cycles, and the similarities between the cycles, the latter due to an uniform selection of characteristics representative of the cycles (6 features per cycle). Finally, the application implements mathematical processes for the purpose of linking to cardiovascular health issues.

William Mateus, Marco Paluszny, Freddy Hernande
Universidad Nacional de Colombia
Cl. 59a #63-20, Medellín, Antioquia
wimateusav@unal.edu.co, mpalusznykl@unal.edu.co, fhernanb@unal.edu.co

PP1
Gpu-Based Approximate Bayesian Computation Algorithms for Network Reverse-Engineering

Elucidating gene regulatory network is an important step towards understanding the normal cell physiology and complex pathological phenotype. Reverse-engineering consists in using gene expression over time or over different experimental conditions to discover the structure of the gene network in a targeted cellular process. The fact that gene expression data are usually noisy, highly correlated, and have high dimensionality explains the need for specific statistical methods to reverse engineer the underlying network. Among known methods, Approximate Bayesian Computation (ABC) algorithms have not been thoroughly studied for network inference. Due to the computational overhead their application is also limited to a small number of genes. Not only have we developed a method that have less computational cost but also have we accelerated that new multi-level ABC approach by using GPUs. At the first level, the method captures the global properties of the network, such as scale-freeness and clustering coefficients, whereas the second level is targeted to capture local properties, including the probability of each couple of genes being linked. Our approach is evaluated on longitudinal expression data in Escherichia coli.

Myriam Maumy-Bertrand
Universite de Strasbourg
IRMA
mmaumy@math.unistra.fr

Frederic Bertrand
Universite de Strasbourg
fbertran@math.unistra.fr

PP1
Finding Circles in High Dimensional Data

In certain data sets, circular structures are known to exist but may require a change of basis to reveal themselves. We present a modification of the projection pursuit algorithm that seeks out two dimensional projections that are near circular. We analyze the case where the circle is sampled uniformly, demonstrate how Newton's root finding algorithm can be used to find projections that have the desired moments, and show how this can be modified to be used in the case where circles are not uniformly sampled, or are given volume. We show how our method can be used in spectral embeddings of graphs with circular structures, and demonstrate the ability to recover a known circle in image patch data.

Brad Nelson
Stanford University
bjnelson@stanford.edu

Geoffrey D. Sanders
Center for Applied Scientific Computing
Lawrence Livermore National Lab
sanders29@llnl.gov

PP1
A Distributed and Incremental SVD Algorithm for Agglomerative Data Analysis on Large Networks

We show that the SVD of a matrix can be constructed efficiently in a hierarchical approach. The proposed algorithm is proven to recover the singular values and left singular vectors of the input matrix A if its rank is known. Further, the hierarchical algorithm can be used to recover the d largest singular values and left singular vectors with bounded error. It is also shown that the proposed method is stable with respect to roundoff errors or corruption of the original matrix entries. Numerical experiments validate the proposed algorithms and parallel cost analysis.

Benjamin W. Ong
Michigan Technological University
ongbw@mtu.edu

Mark Iwen
Michigan State University

markiwen@math.msu.edu

PP1

Multiscale Plasma Modeling: Coupling the Vlasov-BGK Equation and Molecular Dynamics

The heterogeneous multiscale method (HMM) provides a formal structure for constructing multiscale models of systems with scale separation. It has been particularly useful in developing multiphysics models, which typically make scale separation explicit. In this talk, I present a proof of concept of HMM as a modeling method for hot plasma. Molecular dynamics offers a fully detailed model for ionic motion. On the other hand, the Bhatnagar-Gross-Krook (BGK) approximation of the Boltzmann equation is an effective kinetic model for hot plasma given accurate relaxation parameters. The unknown relaxation parameters can be inferred from data collected in short, small molecular simulations, and subsequently used in the kinetic model. Simulations using the hybrid kinetic-molecular dynamic model are both more accurate than the kinetic model alone, and orders of magnitude more efficient than the molecular dynamics model alone. I will present the theory and results, comment on the advantages and limitations of the method, discuss potential applications, and propose future avenues inquiry into multiscale plasma methods.

Jacob Price
University of Washington
jrp14@uw.edu

Gil Shohet
Stanford University
shohet@stanford.edu

Jeffrey Haack, Mathieu Marciante
Los Alamos National Laboratory
haack@lanl.gov, mmarciante@lanl.gov

Michael Murillo
Michigan State University
murillom@msu.edu

PP1

A Conservative Lagrangian-Eulerian Finite Volume Approximation Method for Balance Law Problems

We propose a simple and fast numerical method based on a Lagrangian-Eulerian framework for numerically solving nonlinear balance law problems [E. Abreu, et al., 2017, E. Abreu, et al., 2015]. The hyperbolic part of balance law is written in a space-time divergence form so that the inherent conservation properties of the hyperbolic operator are used efficiently to build a numerical method to hyperbolic balance law problems [J. Douglas, et al., 2000]. Such framework presents an interesting property of being rather independent of a particular structure of the flux function as well as of the source terms. Without any strong restriction over the source term other than integrability on the finite volume, the above procedure leads to a first-order three-point numerical scheme. To enhance resolution and accuracy of the approximations, we make use of polynomial reconstruction ideas into the Lagrangian-Eulerian novel approach. Besides, we use the novel technique to a wide range of nonlinear balance laws that appear in transport in porous media problems as well as to the shallow water equations with discontinuous source term. In such problems, we present evidences that we are calculating qualita-tively correct approximations with accurate resolution of small perturbations around the stationary solution. Verification of the technique is also made by comparison with analytical solutions when they are available.

John Alexander P. Sepulveda
ITM-Institución Universitaria
Medellín-Antioquia-Colombia
jhonperez@itm.edu.co

Eduardo Abreu
University of Campinas - UNICAMP
eabreu@ime.unicamp.br

Arthur Santo
University of Campinas
Campinas-Brazil
arthurmes@gmail.com

PP1

Implementing Parallel Numerical Procedures for 3+1 Fluid Flow Simulations Using Petsc

The objective of this study is to implement parallel numerical procedures for fluid flow applications. In computational fluid dynamics (CFD), problems often result in stiff matrices which are suited to iterative linear solvers. We employ the Portable, Extensible Toolkit for Scientific Computation (PETSc) with Krylov Subspace (KSP) methods and preconditioners (PC) to solve these stiff problems. In particular, we simulate the fluid flow of counter-rotating vortex pairs using both PETSc KSP solvers and an implicit Gauss-Seidel (GS) solver. Grid size, Mach number, and Reynolds number are varied to investigate the effects on the simulation results. The data indicate that PETSc offers improvements in efficiency and robustness.

Jung-Han Kimn, Nicholas Stegmeier
Mathematics & Statistics
South Dakota State University
jung-han.kimn@sdstate.edu,
nicholas.stegmeier@sdstate.edu

Jeffrey Doom
Mechanical Engineering
South Dakota State University
jeffrey.doom@sdstate.edu

PP1

Black-Box Kernel-Level Performance Modeling for Tuning DG on GPUs

We present a mechanism to symbolically gather performance-relevant operation counts from numerically-oriented subprograms ("kernels") expressed in the Loopy programming system, and apply these counts in a simple, linear model of kernel run time. We use a series of "performance-instructive" kernels to fit the parameters of a unified model to the performance characteristics of GPU hardware from multiple hardware generations and vendors. We evaluate predictive accuracy on a broad array of computational kernels relevant to scientific computing, and demonstrate its ability to determine which configuration of a differentiation kernel for a discontinuous Galerkin application performs best. In terms of geometric mean, our simple, vendor- and GPU-type-independent model achieves relative accuracy comparable to that of

previously published work using hardware specific models.

James Stevens, Andreas Kloeckner
University of Illinois
jdsteve2@illinois.edu, andreask@illinois.edu

PP1
Eulerian Versus Lagrangian Data Assimilation

Data assimilation is a process by which a physical model and observational data are combined to produce a more accurate estimate of the state of a system. It is often used when uncertainty (e.g., noise) is present in the systems evolution or in the observational data. For these types of systems, numerical methods must quantify this uncertainty in addition to estimating the mean behavior of the system. Examples of the successful application of data assimilation include predicting weather patterns and ocean currents. We apply a specific data assimilation technique, the Kalman Filter, to estimate a velocity field. We demonstrate how blending a model with data allows us to infer the state of the system with better accuracy than either the model or the data alone would provide. We simulate the estimation of flow fields with different types of observers (floating versus fixed in space) and observational data (position versus velocity measurements) to analyze the effects this has on estimation skill.

Diego A. Rios
NJIT
dar38@njit.edu

Tadanaga Takahashi
New Jersey Institute of Technology
tt73@njit.edu

PP1
Application in the Shiny Library of R for the Estimation of the Linear Mixed Model to Longitudinal Data

The linear mixed model was proposed by Laird and Ware in 1982, since this time it has been very useful, due to the versatility to analyze grouped data and longitudinal data from clinical and socio-economic studies [West et al, Linear mixed models, a practical guide using Statistical Software, 2007]. This model has a fixed effects component and two random components, effect and random error, which are assumed to come from a normal distribution and that have constant variance, however these assumptions are not always fulfilled, which alters the inferences about the Parameters, goodness of fit indicators and possible predictions [Fitzmaurice et al, Applied Longitudinal Analysis, 2011]. In the literature it is possible to find several data sets with a departure from the normality assumptions in the random component, so that in this article proposed an interactive application using the Rstudio IDE and its shiny library to estimate the linear mixed model using different databases, in addition the normality is assessed in the random component with the test of Zhang and Davidian [Linear Mixed Models with Flexible distribution of random effects for longitudinal data, 2001].

Johanna T. Trochez Gonzalez
Universidad Nacional de Colombia
jtrochezg@gmail.com

Juan Carlos Salazar
UNIVERSIDAD NACIONAL DE COLOMBIA
jcsalaza@unal.edu.co

Freddy Hernandez
Universidad Nacional de Colombia
fhernanb@unal.edu.co

Marisol Valencia
Tecnológico de Antioquia
solmarival@gmail.com

PP1
Discrete Data Analytic Study of the Traffic Light Problem

It is clear as technology and humanity continues to advance, the role of traffic also grows. As such, we continue to push our understanding of traffic, we derived an algorithm to predict an individual's most likely path of travel from point A to point B by solving a system of non-linear differential equations. Data were collected randomly on a local neighborhood about the different attributes of paths in contrast to the varying driving conditions. Finally we tested and compared the analytic model with a proposed ideal abstract graph theoretic model.

Mathew K. Tucker
STUDENT
mktuck8914@ung.edu

Bikash Das
University of North Georgia
bikash.das@ung.edu

Amrita Acharyya
University of Toledo
amrita.acharyya@utoledo.edu

PP1
Extend Levelt's Propositions to Multistable Binocular Rivalry

Binocular rivalry has been used as a tool to study cortical mechanisms lying under visual awareness. While a huge body of literature devoted to bistable binocular rivalry (rivalry between two images), only a handful of works investigated multistable (more than two states) binocular rivalry. In this study, we showed experimentally and numerically that the well-known Levelts Propositions, which characterize dynamic features of bistable rivalry, can be extended to multistable case.

Yunjiao Wang
Department of Mathematics
Texas Southern University
wangyx@tsu.edu

Alain Jacot-Guillarmod
Lausanne University Hospital
Switzerland
aljacot@gmail.com

Claudia Pedroza
The University of Texas
claudia.pedroza@uth.tmc.edu

Haluk Ogmen
University of Denver
ogmen@central.uh.edu

Zackary Kilpatrick
University of Colorado
zpkilpat@colorado.edu

Kresimir Josic
University of Houston
Department of Mathematics
josic@math.uh.edu

PP1

Double-Exposure Epidemiological Model

We investigate a plausible model for a contagion that spreads only after double-exposure; in other words, two "infected' connections are necessary before the disease may spread to a "susceptible' individual. Solutions to a differential equation model are compared to results from network simulations. The model is further generalized to the n-exposure case, and the resulting delay in dynamics is analyzed. We posit that although the literal case of disease spread may be hypothetical, the spread of opinions may be well explained by this model. This research was performed in collaboration with an undergraduate student, as a senior thesis project.

Haley Yaple, Kerry Stapf
Carthage College
hyaple@carthage.edu, kstapf@carthage.edu

PP1

Modeling Shape Dependent Mott Oxidation of Nanosized Metal Particles

We describe analytic and numerical results for modeling Mott oxidation of nospherical nanosized aluminum particle. Our results include existence of local solutions for a nonlinear generalization of Hele Shaw moving boundary problem, and numeric simulations using subsolution and mapping methods. Those results provide an estimate of oxidation time of nonspherical aluminum nanosized particles, and have important applications in modeling nano-energetic materials, composed of mixtures of nano-sized aluminum and oxidizer particles, with superior performance in highly energetic applications.

Maxim Zyskin
School of Mathematical Sciences, University of Nottingham
maxim.zyskin@nottingham.ac.uk

Karen Martirosyan
University of Texas, Rio Grande
karen.martirosyan@utrgv.edu

PP2

AWM Workshop - Tailoring Tails in Taylor Dispersion: How Boundaries Shape Chemical Deliveries in Microfluidics

We present a study of the dispersion of a passive scalar in laminar shear flow through rectangular and elliptical channels. Through asymptotic analysis, Monte Carlo simulations and laboratory experiments, we show that the channels cross-sectional aspect ratio sets the longitudinal asymmetry of the tracer distribution at long time: thin channels generate distributions with sharp fronts and tapering tails, whereas thick channels produce the opposite effect. Potential applications to microfluidics will be discussed.

Francesca Bernardi
UNC
bernardi@live.unc.edu

PP2

AWM Workshop - A New Goal-Oriented A Posteriori Error Estimation for 2D and 3D Saddle Point Problems in Hp Adaptive Fem

We present a new approach on goal-oriented a posteriori error estimation for an automatic hp-Adaptive Finite Element Method. The method is based on the classical dual-weighted algorithm on local patches and applying the Clment type interpolation operators. The reliability and also the efficiency of the proposed a posteriori error estimator have been proved. Finally, the performance of the proposed estimator for both h- and hp-Adaptive FEM has been investigated in numerical examples for Saddle point problem.

Arezou Ghesmati
Texas A&M University
aghesmati@math.tamu.edu

PP2

AWM Workshop - An Invariant-Region-Preserving Limiter for DG Method to Compressible Euler Equations

We introduce an explicit invariant-region-preserving limiter for compressible Euler equations. The invariant region considered consists of positivity of density and pressure and a maximum principle of a specific entropy. The reconstructed polynomial preserves the cell average, lies entirely within the invariant region and does not destroy the high order of accuracy for smooth solutions. Numerical tests are presented to illustrate the properties of the limiter. In particular, the tests on Riemann problems show that the limiter helps to damp the oscillations near discontinuities.

Yi Jiang
Iowa State University
yjiang1@iastate.edu

Hailiang Liu
Iowa State University
USA
hliu@iastate.edu

PP2

AWM Workshop - Sobolev Discontinuous Galerkin (dG) Methods

The dG method is a popular polynomial-based method known for its spectral accuracy and geometric flexibility. Despite its nice properties, dG suffers from a restrictive time step size. In this talk, we present Sobolev dG, a novel dG method that allows for much larger time steps compared to traditional dG methods, with computational results illustrating Sobolev dGaAZs excellent time stepping properties. Sobolev dG tests with low degree polynomials while maintaining the accuracy of high-order polynominals

Adeline Kornelus
University of New Mexico

kornelus@unm.edu

PP2
AWM Workshop - Computational Approaches for Linear Goal-Oriented Bayesian Inverse Problems

We present a comparison of different approaches for computing low rank approximations to posterior covariances arising in goal-oriented inverse problems. In particular, we study problems where both the forward model and the quantity of interest depend linearly on the uncertain parameters. We present and compare algorithms for the computation of optimal approximations, referring to recent work where the approximations are obtained as low rank updates to the priors.

Karina Koval
Courant Institute of Mathematical Sciences
koval@cims.nyu.edu

PP2
AWM Workshop - An AMG Approach in Solving Graph Laplacians of Protein Networks Based on Diffusion State Distance Metrics

In this presentation, protein networks from 2016 Disease Module Identification DREAM Challenge are analyzed. We redefined the Protein-Protein Interaction networks on a new distance metric, "Diffusion State Distance' metric, and applied a modified Algebraic Multi-grid Method to calculate the distance between each pair of nodes. Finally, we applied spectral clustering to partition the protein network into functional modules. Consequently, we ranked No.1 out of over 50 teams over the world.

Junyuan Lin
Tufts University
junyuan.lin@tufts.edu

PP2
AWM Workshop - Polynomial Preconditioned Arnoldi for Eigenvalues

Polynomial preconditioning has been explored for Krylov methods for large eigenvalue problems but has not become standard, possibly due to difficulty in obtaining a helpful polynomial. We give a simple choice for a polynomial preconditioner and a stable way to compute with it. When applied to the Arnoldi method for eigenvalues, this approach can significantly reduce computational costs for difficult problems.

Jennifer A. Loe, Ron Morgan
Baylor University
jennifer_loe@baylor.edu, Ronald_Morgan@baylor.edu

Mark Embree
Department of Mathematics
Virginia Tech
embree@vt.edu

PP2
AWM Workshop - Hyperspectral Image Classification Using Parallellized Graph Clustering Methods

We introduce two data classification algorithms and investigate many-core node parallelization schemes. The new algorithms are derived from PDE solution techniques and they provide a significant performance and accuracy advantage over traditional data classification algorithms. We use OpenMP as the parallelization language to parallelize the most time-consuming parts of the algorithms and then optimize the OpenMP implementations. We show performance improvement and strong scaling behavior.

Zhaoyi Meng
University of California, Los Angeles
mzhy@ucla.edu

PP2
AWM Workshop - A Reaction-Diffusion Model for Cell Polarization in Yeast

Cell polarization is fundamental to cellular processes such as differentiation, migration, and development. We consider cell polarization driven by a pheromone gradient in mating yeast. This is modeled by a large reaction-diffusion system. Many parameters in the system can be only crudely estimated, which leads to inaccuracy in the model. The aim of our work is to determine the sensitivity of the system to the parameters and perform data-driven parameter estimation.

Marissa Renardy
The Ohio State University
renardy.1@osu.edu

PP2
AWM Workshop - Band-Edge Solitons in the Nls Equation with Periodic Pt-Symmetric Potentials

The bifurcation of nonlinear bound states from the spectral edges of the NLS equation with periodic parity-time (PT)-symmetric potentials is studied asymptotically and computationally. These modes undergo a transition near the breakdown point of the PT symmetry. The effective mass tensor and nonlinear coupling constants, which determine the structure of these modes, are analyzed in detail. The implication to collapse dynamics is discussed.

Jessica Taylor
University of California, Merced
jtaylor5@ucmerced.edu

PP2
AWM Workshop - Almost Sure Convergence of Particle Swarm Optimization Using Pure Adaptive Search Method

Particle swarm optimization (PSO) is a population based stochastic optimization method, which has been used across a wide range of applications. Though there have been several studies about the convergence of PSO, the convergence proofs in these studies are either imprecise or under unrealistic assumptions. Here, we present a almost surely convergence analysis of PSO based on the fact that particles personal and global best values follow pure adaptive search method.

Ganesha Weerasinghe
Auburn University

ksw0013@auburn.edu

PP3
How Many Dimensions Is *high* Dimensions?

Minisymposterium: How many dimensions is *high* dimensions?

Izabel P. Aguiar, Jessica R. Deters
Colorado School of Mines
iaguiar@mines.edu, jdeters@mines.edu

PP3
Active Subspaces: Emerging Ideas in Dimension Reduction for Parameter Studies

Active subspaces are part of an emerging set of subspace-based dimension reduction tools that identify important directions in the input parameter space.

Paul Constantine
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu

PP3
Inverse Regression for Ridge Recovery

We investigate the mathematical implications of applying sufficient dimension reduction (SDR) to deterministic functions. In this context, SDR provides a framework for ridge recovery. A function exhibiting ridge structure may be expressed as another function (or ridge profile) of fewer inputs. SDR lays the foundation for algorithms that search for the optimal subspace, called the central ridge subspace, spanning these reduced inputs. We examine two inverse regression methods, sliced inverse regression (SIR) and sliced average variance estimation (SAVE), that approximate this subspace. We provide convergence results for these algorithms towards solving the ridge recovery problem.

Andrew Glaws
Colorado School of Mines
aglaws@mines.edu

Paul Constantine
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu

Dennis Cook
University of Minnesota
dennis@stat.umn.edu

PP3
Parameterization-Independent Active Subspaces of Engineering Geometries

Design and optimization applications benefit from understanding the dependency of a quantity of interest on a set of independent parameters. Approximating active subspaces offers analytic insights for characterizing the dependency between parametric representations and quantities of interest. A popular test problem involves the parameterization of airfoil shapes in a transonic flow field. Of the variety of possible parametric representations for airfoil shapes, basis expansion interpretations allow for easy manipulation and adaptation of any proposed parameterization. We discuss how half-power polynomial series basis expansion parameterizations can be related to physically relevant airfoil quantities. By incorporating active subspaces, it is possible to identify reduced dimension approximations of transonic lift and drag that can be related to physically intuitive airfoil shape quantities. We discuss obtaining and interpreting an accurate two dimensional approximation of both transonic lift and drag to inform a multi-objective problem.

Zach Grey
Colorado School of Mines
zgrey@mymail.mines.edu

Paul Constantine
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu

PP3
Data-Driven Polynomial Ridge Approximation Using Variable Projection

Inexpensive surrogates are key for reducing the cost of complex engineering problems. Ridge approximations are one class of surrogates that mimic the behavior of the original function but act only on a low-dimensional subspace of the input domain. Here we introduce a new, fast algorithm for constructing polynomial ridge approximations from function samples in a least squares sense. Naively, this requires optimizing both the polynomial coefficients and the subspace. However, noting that given a fixed subspace, the polynomial coefficients are given by a linear least squares problem, we implicitly solve for these coefficients using Variable Projection. This leaves an optimization problem over the subspace alone. Here present an algorithm that finds the optimal subspace by optimizing over Grassmann manifold using a Gauss-Newton Hessian approximation. Our result improves on existing algorithms for polynomial ridge approximation, yielding surrogates four thousand times faster that converge to near machine precision. This result provides better surrogate models for engineering problems and the improved speed allows frequent updating of the surrogate as more samples are added.

Jeffrey M. Hokanson
Colorado School of Mines
hokanson@mines.edu

Paul Constantine
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu

PP4
Using Parameter Estimation Techniques to Analyze a Mathematical Wound Healing Model

Since the medical treatment of diabetic foot ulcers remains a challenge for clinicians, a quantitative approach using de-identified patient data and mathematical modeling can help researchers understand the physiology of the wounds. The goal of this project is to utilize individual patient data to identify key parameters, through the use of nonlinear mixed effects modeling, and delayed rejection adaptive metropolis (DRAM), in the healing process in order to improve patient care and diagnosis. In this work, we plan to

use nonlinear mixed effects modeling to attribute wound healing variability to either fixed effects, parameters that are more likely to remain constant for all patients, or random effects, parameters that vary from patient to patient. The identified random effects should then be taken into special consideration when treating patients with chronic wounds, especially diabetic foot ulcers. A Bayesian approach using DRAM, a MATLAB implementation of a Metropolis-Hastings algorithm, will also be used to estimate and analyze parameters. Using DRAM can help with parameter estimation since the available data is sparse and can help find parameter identifiability issues.

Rachel N. French, Rachel Turner, Jacob Menix
Western Kentucky University
rachel.french786@topper.wku.edu,
rachel.turner937@topper.wku.edu, jacob.menix841@topper.wku.edu

PP4
Patterns in the Starch-Iodine Reaction

The reaction between starch and iodine has interested people since 1812, including a young chemically intrigued Alan Turing. The interaction of iodine vapor with a starch solution can produce a variety of patterns such as stripes and hexagons. A model to explain this reaction which makes use of the cooperative binding of iodine molecules to the starch helix will be presented.

Derek Handwerk
Colorado State University
handwerk@math.colostate.edu

PP4
Offline-Enhanced Reduced Basis Method through Adaptive Construction of the Surrogate Parameter Domain

The Reduced Basis Method (RBM) is a popular certified model reduction approach for solving parametrized partial differential equations. However, the large size or high dimension of the parameter domain leads to prohibitively high computational costs in the offline stage. In this work we propose and test effective strategies to mitigate this difficulty by performing greedy algorithms on surrogate parameter domains that are adaptively constructed. We propose two ways to construct the surrogate parameter domain, one inspired by inverse transform sampling for nonstandard univariate probability distributions and the other based on the Cholesky Decomposition of an error correlation matrix. These algorithms are capable of speeding up RBM by effectively alleviating the computational burden in offline stage without degrading accuracy, assuming that the solution manifold has low Kolmogorov width. We demonstrate the algorithm's effectiveness through numerical experiments.

Jiahua Jiang
University of Massachusetts, Dartmouth
jjiang@umassd.edu

Yanlai Chen
Department of Mathematics
University of Massachusetts Dartmouth
yanlai.chen@umassd.edu

Akil Narayan
University of Utah
akil@sci.utah.edu

PP4
A Parametric Level-set Method for Partially Discrete Tomography

Partially discrete images consist of a continuously varying background and an anomaly with a constant (known) grey-value. Such images occur in many applications, including, medical imaging and electron microscopy. To incorporate prior information about the anomaly in the reconstruction, we represent its geometry using a level-set function, parametrized by radial basis functions (RBF). We pose the reconstruction problem as a bi-level optimization problem in terms of the background and the RBF coefficients. To constrain the background reconstruction we impose smoothness through Tikhonov regularization. The bi-level optimization problem is solved in an alternating fashion; in each iteration we first reconstruct the background and consequently update the level-set function. With limited data, our method successfully reconstructs the anomaly, outperforming several other algorithms for partially discrete tomography.

Ajinkya Kadu
Mathematical Institute, Utrecht University, The Netherlands
a.a.kadu@uu.nl

Tristan van Leeuwen
Mathematical Institute
Utrecht University
t.vanleeuwen@uu.nl

K. Joost Batenburg
Centrum Wiskunde & Informatica, Amsterdam
joost.batenburg@gmail.com

PP4
Pattern Formation of a Nonlocal, Anisotropic Interaction Model

We consider a class of interacting particle models with anisotropic repulsive-attractive interaction forces whose orientations depend on an underlying tensor field. An example of this class of models is the so-called Kcken-Champod model describing the formation of fingerprint patterns. This class of models can be regarded as a generalization of a gradient flow of a nonlocal interaction potential which has a local repulsion and a long-range attraction structure. In contrast to isotropic interaction models the anisotropic forces in our class of models cannot be derived from a potential. The underlying tensor field introduces an anisotropy leading to complex patterns which do not occur in isotropic models. This anisotropy is characterized by one parameter in the model. We study the variation of this parameter, describing the transition between the isotropic and the anisotropic model, analytically and numerically. We analyze the equilibria of the corresponding mean-field partial differential equation and investigate pattern formation numerically in two dimensions by studying the dependence of the parameters in the model on the resulting patterns. Based on these theoretical and numerical results we adapt the forces in the Kcken-Champod model in such a way that we can model fingerprint patterns (and more general any desired pattern) as stationary solutions.

Lisa Maria Kreusser
University of Cambridge

L.M.Kreusser@damtp.cam.ac.uk

Martin Burger
University of Muenster, Germany
martin.burger@wwu.de

Bertram Düring
University of Sussex
b.during@sussex.ac.uk

Peter A. Markowich
University of Cambridge
p.a.markowich@damtp.cam.ac.uk

Carola-Bibiane Schönlieb
DAMTP, University of Cambridge
cbs31@cam.ac.uk

PP4
Mathematical and Computational Modelling of Compressible Non-isothermal Viscoelastic Flow

Compressible and non-isothermal effects are often ignored when modelling flows of non-Newtonian fluids. The additional equations governing density and temperature transport increase the complexity of the governing system of nonlinear partial differential equations which adds to the challenge of devising efficient and stable numerical schemes. Taylor-Galerkin pressure correction schemes coupled with Discrete Elastic Viscous Stress Splitting (DEVSS) stabilisation enable accurate solutions to be generated for a wide range of viscosities and relaxation times. The derivation of the governing equations is described and some numerical results on benchmark problems are presented. In particular, the flow between eccentrically rotating cylinders (the journal bearing problem) is considered for a range of relaxation times and the influence of compressibility and viscoelasticity on torque and load bearing capacity is assessed.

Alex Mackay
Cardiff University
mackaya1@cardiff.ac.uk

PP4
Modelling a District Heating Network, Gas Network and Power Grid as an Integrated System

Energy network systems are usually modelled as separate systems in their own right, i.e. as a district heating network, a gas network or a power grid. In order to improve the design and operations of the energy systems there is, however, an increasing demand to model these networks in combination in an integrated system. We investigate the possible ways of coupling the networks and integrating the networks into a single integrated model. The focus of the research is to integrate networks on a regional scale, meaning that the distribution network of each energy carrier is considered.

Anne S. Markensteijn
Delft University of Technology
A.S.Markensteijn@tudelft.nl

PP4
Kernel-based Reconstruction of Spatially Embed-ded Complex Networks

With increasing supply of data collected from numerous complex systems, a key question is what patterns and properties of the underlying systems can be extracted from such data. A particular such problem is to infer the network structure of interacting components from data, mathematically formulated as an inverse problem. Given that numerous complex networks in real-life are spatially embedded, we ask, can such spatial constraints be exploited (rather than suffered from) to make better inference? An example is the synaptic connections in human brains, which are mostly short-range and have profound impacts on brains neurological dynamics and functionality. Based on the preference of short-range spatial connections, we develop a kernel-based Lasso framework to infer complex spatial networks. We show by numerical experiments that the proposed method improved significantly upon existing network inference techniques. Importantly, such enhancement is achieved even when the exact spatial distribution of the embedded edges is unknown, making the method particularly relevant as a computational tool to efficiently and reliably infer large spatial networks in practice.

Fernando J. Quevedo
Department of Mathematics
Clarkson University
QuevedFJ@Clarkson.edu

Erik Bollt
Clarkson University
bolltem@clarkson.edu

Jie Sun
Mathematics
Clarkson University
sunj@clarkson.edu

PP4
A Decision Tree Classification Model to Identify Flight Delay Patterns of U.S. Airlines

Flight disruptions and cancellations are inevitable part of commercial air travel, costing the travel industry up to an estimated \$60 billion annually, equating to 8% of global industry revenues. From 2008 to date, on average, about 19% of flights were delayed at departure. 26% of flight departures were at Chicago OHare, 25% of which were AA flights. In this project, we present a decision tree model to identify the flight delay patterns and significant factors that can accurately predict flight departure delays. To achieve this we apply machine learning techniques to a large-scale flight data, containing 6412 American Airlines flights from Chicago O'Hare International Airport in 2008, extracted from American Statistics Association. We first use linear regression to identify the most important factors affecting delays. Subsequently, we use different classifiers, SVM, Logistic Regression, Decision Tree, Naive Bayes, and Nearest Neighbor, to predict delay and make comparison between the classifiers through 10x10 folding cross validation accuracy. We present a logistic regression model with 95% accuracy and C4.5 Decision Tree classification model with an accuracy about 91%. The results obtained can be used for proposing a multi-objective optimization model for minimizing flight delays and associated costs, taking the significant variables affecting the flight delay as constraints.

Nandini Rakala, James Williams, Willa Huddleston
Florida Institute of Technology

nrakala2015@my.fit.edu, jameswilliam2014@my.fit.edu, whswim@yahoo.com

Munevver Subasi
Florida Institute of Technology
Department of Mathematical Sciences
msubasi@fit.edu

PP4

Modeling Flow and Fouling in Membrane Filters: Insights into Filter Design

Membrane filters are in widespread use, and manufacturers have considerable interest in improving their performance, in terms of particle retention properties, and total throughput over the filter lifetime. A good question to ask is therefore: what is the optimal configuration of filter membranes, in terms of internal morphology (pore size and shape), to achieve the most efficient filtration? To answer this question, we must first propose a robust measure of filtration performance. As filtration occurs the membrane becomes blocked, or fouled, by the impurities in the feed solution, and any performance measure must take account of this. For example, one performance measure might be the total throughput (the volume of filtered feed solution) at the end of the filtration process, when the membrane is so badly blocked that it is deemed no longer functional. In this work we present a simplified mathematical model, which (i) characterizes membrane internal pore structure via pore or permeability profiles in the depth of the membrane; (ii) accounts for various membrane fouling mechanisms (adsorption, blocking and cake formation); and (iii) predicts the optimum pore profile for our chosen performance measure.

Pejman Sanaei
New Jersey Institute of Technology
ps468@njit.edu

PP4

Generic Steady State Bifurcations in Homogeneous Coupled Cell Networks

Rink, Sanders and Nijholt have provided numerous results on dynamics in homogeneous coupled cell networks. Using their methods, one can present network ODEs as (subsystems of) systems that are symmetric with respect to a monoid representation. This draws attention to very exciting generalizations of representation theory and equivariant dynamics. We investigate this generalization and especially the question of generic steady state bifurcations and their possible locations which could up to now only partly be answered: either in the direct context of the networks or in a special case of the monoid representation. We aim at generalizing this last statement to include more general representations. This type of result has the advantage of providing information on the dynamics of classes of networks rather than individual ones as the results hold for all those networks connected to the same monoid representation. By employing methods from equivariant bifurcation theory of groups on the one hand and the theory of monoid representations on the other we can extend the bifurcation result to special types of monoids and to more types of monoid representations.

Sören Schwenker
University of Hamburg

soeren.schwenker@uni-hamburg.de

PP4

Global Recurrence Relations of Epidemiological Cellular Automata

Cellular automata (CA) models are a relatively simple discrete method that can be used to simulate complicated models such as the spatial spread of a disease where there is a fixed radius controlling the infectivity of individuals. The relative ease of CA implementation is counterbalanced by the difficulty of performing rigorous analysis for any emergent behavior. Calculating fixed-point stability, analyzing parameter sensitivity, and fitting parameters to data becomes computationally expensive. Previous work has been performed using mean-field theory to develop approximate global solutions for probabilistic CA with von Neumann neighborhoods on a finite lattice. We extend this notion to develop a framework for approximating cell densities of a probabilistic epidemiological CA model with fixed radius neighborhoods and random walk cell mobility. Using this framework, we develop a 2-dimensional recurrence formula. The analytic methods for this complicated model then reduces to methods similar to those performed on systems of compartmental ODE SIR models for the spread of a disease.

Michael Yereniuk
Worcester Polytechnic Institute
mayereniuk@wpi.edu

PP5

Creating Art with Mathematical Symmetries

In this project, we constructed complex-valued functions invariant with respect to rotations and lattices and we visualized them using the domain-coloring algorithm and a software.

Carmen Acosta-Alonzo, Kenyona Bethea
Bennett College
Carmen.acosta@bennett.edu,   kenyona.bethea@bennett.edu

PP5

Why Do They Not Believe?: The Network Dynamics of Opinion

Convention assumes that with greater access to information, logic will lead everyone to the same conclusions, but this is not the case. Even with access to information sources such as the internet, recent years have not seen a greater acceptance of opposing ideals, but rather the opposite. Polls show opinions becoming extreme rather than converging to the center, and partisanship in the bodies of government has become the norm. In such a context of growing social and political division in the American community and abroad, we show how idea transmission can be understood through the lens of evolutionary dynamics. We assume nothing about the validity of the ideas in question, or the logical thinking of human actors, but rather let all changes within a network of believers and disbelievers be based on a fitness function that takes into account the relationship between a node's opinion and the opinions of its neighbors. As beliefs spread during successive time steps, we consider how the presence of those ideas can influence the underlying network structure and ultimately coevolve

with it.

Tucker E. Evans
Dartmouth College
tevans1080@gmail.com

PP5

Construction of 3D Representations for Small-Sized, Detailed Objects With Perspective Limitations: A Case Study

With the steady growth of various applications that can take advantage of 3D representations of objects such as virtual reality, it is important to expand the pool of representable items. Items that have been particularly difficult to reconstruct from currently existing 3D reconstruction applications include inaccessible small-sized objects with finer details, smooth featureless, surfaces, and objects with having perspective limitations. An object with a perspective limitation is defined as an object that lacks the capacity to be viewed along any complete, rotational axis inside the 3D space. In this particular case study, the target object is human teeth in situ. The creation of a unique 3D representation of this object is attempted by editing a pre-existing, perfect model (obj. file) using the Java 3D package. The model and its smaller components can be modified by coding specific edits such as the translational or rotational movement of a tooth. The anticipated use of the final product is a mobile health application designed to accurately represent the users teeth and gums for monitoring oral health. Specifically this custom 3D model of a childs teeth will be used to detect and address areas of demonstrate locations of bacterial growth leading to caries, and where therapy needs to be applied at home by a parent. Our hypothesis is an accurate 3D model will invoke more effective are and treatment either by the caregiver client or the user.

Hae In Lee
University of Washington
haeinalee@gmail.com

Figure courtesy Fabio Fagnani.

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SP1

AWM-SIAM Sonia Kovalevsky Lecture: Mitigating Uncertainty in Inverse Wave Scattering

Inverse wave scattering is an inverse problem for the wave equation, driven by a broad spectrum of applications. It is an interdisciplinary area that involves mathematical analysis, computational modeling, statistics and signal processing. This lecture will discuss one important challenge due the uncertainty of the model for inversion. Uncertainty is unavoidable in applications, not only because of noise, but because of lack of detailed knowledge of complex media through which the waves propagate.

Liliana Borcea
University of Michigan
borcea@umich.edu

SP2

The Jon von Neumann Lecture: Singular Perturbations in Noisy Dynamical Systems

Consider a deterministic dynamical system in a domain containing a stable equilibrium, e.g., a particle in a potential well. The particle, independent of initial conditions eventually reaches the bottom of the well. If however, a particle is subjected to white noise, due, e.g., to collisions with a population of smaller, lighter particles comprising the medium through which the Brownian particle travels, a dramatic difference in the behavior of the Brownian particle occurs. The particle can exit the well. The natural questions then are: how long will it take for it to exit and from where on the boundary of the domain of attraction of the equilibrium will it exit. We compute the mean first passage time to the boundary and the probability distribution of boundary points being exit points. When the noise is small each quantity satisfies a singularly perturbed deterministic boundary value problem.

Bernard Matkowsky
Northwestern Universtiy, USA
b-matkowsky@northwestern.edu

SP3

Past President's Address: The Future of SIAM: Looking to the Mathematicians of Tomorrow

During my tenure as SIAM president, I sought to emphasize that the S in SIAM stands for students by focusing on boosting our global presence and cultivating the next generation of mathematicians. To all the long-time SIAM members, can you guess how many new international chapters weve added since 2012? To all the new SIAM student members weve welcomed in that period, can you name all the ways SIAM can help you grow your careers? At the 2017 SIAM Annual Meeting I will invite our Student Chapters to use their own words to answer these important questions through a series of videos spanning several continents. The advances weve made should make us all proud. Of course, theres always more that SIAM can do as it continues to push ahead in order to remain at the vanguard of the scientific community.

Irene Fonseca
Carnegie Mellon University
Center for Nonlinear Analysis
fonseca@andrew.cmu.edu

SP4

James H. Wilkinson Numerical Analysis and Scientific Computing Prize Lecture: Tensors in Computational Mathematics

We show that in many instances, one would find a higher-order tensor, usually of order three, at the core of an important problem in computational mathematics. The resolution of the problem depends crucially on determining certain properties of its corresponding tensor. We will draw examples from (i) numerical linear algebra: fastest/stablest algorithms for matrix product, matrix inversion, or structured matrix computations; (ii) numerical optimization: SDP-relaxations of NP-hard problems, self-concordance, higher-order KKT conditions; and, if time permits, (iii) numerical PDEs: tensor network ranks. This talk is based on joint works with Ke Ye, with Shenglong Hu, and with Shmuel Friedland.

Lek-Heng Lim
University of Chicago
lekheng@galton.uchicago.edu

SP5

I.E. Block Community Lecture: From Flatland to Our Land: A Mathematicians Journey through Our Changing Planet

Mathematics is central to our understanding of the world around us. We live in a vast dynamical system, the many dimensions of which can be interrogated with mathematical tools. In this talk I will consider our changing climate. I will describe the scientific evidence that tells us how and why our climate is changing, and what the future may hold. In this journey I will pause at various waypoints to describe in more detail some of the insight different branches of mathematics are providing. Diverse examples will include applying ideas from dynamical systems research to create novel strategies for measuring the ocean mixing processes that are critical to the flow of heat and carbon through the Earth system, through to employing statistical learning techniques to improve future predictions of Arctic sea ice, currently in perilous decline. Climate change is one of the greatest challenges facing humanity. Responding to the challenge requires robust scientific evidence to inform policies. Opportunities for mathematicians to contribute to this important issue abound.

Emily Shuckburgh
British Antarctic Survey, United Kingdom
emily.shuckburgh@bas.ac.uk

JP1

Bio-Inspired Dynamics for Multi-Agent Decision-Making

I will present a generalizable framework that uses the singularity theory approach to bifurcation problems, and other tools of nonlinear dynamics, to translate some of the remarkable features of collective animal behavior to an abstract agent-based model. With the abstract model, analysis and design of decision-making between alternatives can be systematically pursued for natural or engineered multi-agent systems. To illustrate, I will apply the framework to explore and extend value-sensitive decision-making dynamics that explain the adaptive and robust behavior of

house-hunting honeybees.

Naomi E. Leonard
Princeton University
naomi@princeton.edu

CP1

On the Hierarchical Risk-averse Control Problems for Diffusion Processes

In this paper, we consider a risk-averse control problem for diffusion processes, in which there is a partition of the admissible control strategy into two decision-making groups (namely, the *leader* and *follower*) with different cost functionals and risk-averse satisfactions. Our approach, based on a hierarchical optimization framework, requires that a certain level of risk-averse satisfaction be achieved for the *leader* as a priority over that of the *follower's* risk-averseness. In particular, we formulate such a risk-averse control problem using partially coupled *forward-backward stochastic differential equations* that allow us to introduce a family of time-consistent dynamic convex risk measures, based on backward-semigroup operators, w.r.t. the strategies of the *leader* and that of the *follower.* Moreover, under suitable conditions, we establish the existence of optimal risk-averse solutions, in the sense of viscosity solutions, to the associated risk-averse dynamic programming equations. Finally, we remark on the implication of our result in assessing the influence of the *leader's* risk-averse satisfaction on the risk-averseness of the *follower* in relation to the direction of *leader-follower* information flow.

Getachew K. Befekadu
Department of Industrial System Engineering
University of Florida - REEF
gbefekadu@ufl.edu

Eduardo Pasiliao
Air Force Research Laboratory
pasiliao@eglin.af.mil

CP1

Convergence of Discrete-time Games to Path-dependent Isaacs Partial Differential Equations with Quadratically Growing Hamiltonians

We consider discrete-time approximations of deterministic differential games with dynamics and costs depending on past histories of state trajectories. Taking into consideration important problem classes such as linear quadratic problems with unbounded controls, we assume that the Hamiltonian and the value functions can be quadratically growing. Modifying the notion of viscosity solutions of Lukoyanov with careful estimates of values and optimal controls, we prove that the discrete-time upper values converge to a unique viscosity solution of the path-dependent Isaacs partial differential equation as the size of the time step goes to 0.

Hidehiro Kaise
Graduate School of Engineering Science
Osaka University
kaise@sigmath.es.osaka-u.ac.jp

CP1

Intrinsic and Apparent Singularities in Differentially Flat Systems, and Application to Global Motion Planning

In this paper, we study the singularities of locally differentially flat systems, in the perspective of providing global or semi-global motion planning solutions for such systems: flat outputs may fail to be globally defined, thus potentially preventing from planning trajectories leaving their domain of definition, the complement of which we call singular. Such singular subsets are classified into two types: apparent and intrinsic. A rigorous defintion of these singularities is introduced in terms of atlas and local charts in the framework of the differential geometry of jets of infinite order and Lie-Bcklund isomorphisms. We then give a criterion allowing to effectively compute intrinsic singularities. Finally, we show how our results apply to the global motion planning of the well-known example of non holonomic car.

Yirmeyahu Kaminski
Department of Applied Mathematics
Holon Institute of Technology
jykaminski@gmail.com

Jean Levine
MinesParisTech
Institute Henri Poincarre
jean.levine@mines-paristech.fr

François Ollivier
Ecole Potytechnique
francoisollivier1@free.fr

CP1

Optimality Conditions for Switching Operator Differential Equations

We consider a framework for optimal switching of hybrid abstract evolution equations. The theory includes time dependent dynamics driven by semilinear partial differential equations of parabolic or hyberbolic type, allowing for the switching of the principal parts over discrete sets of switching modes with possibly discontinuous transition maps. Questions arising are the well-posedness of such systems when varying number and position of switching points and the optimization of switching decisions with respect to a cost functional including switching costs. In this talk, we present first order necessary conditions for optimality with respect to switching times and discuss strategies for optimizing the discrete mode sequence. The results are based on a hybrid adjoint calculus. Points satisfying the optimality conditions can be found using projected descent methods. As an application we consider optimal open/close and on/off switching control of valves and compressors in a gas network modeled by a graph with simplified euler equations on edges and suitable coupling conditions at nodes.

Fabian Rueffler
FAU Erlangen-Nuernberg
Lehrstuhl Angewandte Mathematik 2
fabian.rueffler@fau.de

Falk M. Hante
Friedrich-Alexander-Universitaet Erlangen-Nuernberg
falk.hante@fau.de

CP1

Minimization of the Boundary Energy Functional

with Inequality Constraints for the Wave Equation

We consider the problem to control a vibrating string to rest in a given finite time.The string is fixed at one end and controlled by Neumann or Dirichlet boundary control at the other end. We consider minimization of the boundary energy functional with inequality constraints on boundary control. Previously, the problem of minimizing the energy functional boundary was solved. However, the form of the explicit solution formula difficult to implement technically, because from the energy point of view our control can be divided into three parts: addition energy to the system to extinguish the initial state for a short period of time, then a long wait, and then adding energy to produce the final state to the set time T. We solve the problem of boundary control with a local restriction on adding energy: in any preassigned period of time energy management should not exceed the prescribed constant. We give an explicit representation of the L2-norm minimal control in terms of the given initial state and constant from local boundary energy constraints inequality.

Ilya Smirnov
Lomonosov Moscow State University
Faculty of Computational Mathematics and Cybernetics
reference20031@rambler.ru

CP2

Minimal Realization of Mimo Linear Systems using Hermite Form

Minimal realization is closely related to model reduction. While model reduction is an approximation of a system by a reduced order, minimal realization is an exact order reduction. Minimal realization permits to accurately represent the system with a reduced order. Many minimal realization techniques have been proposed in the past. The proposed method is used to compute the minimal realization of linear time-invariant (LTI) system. It is based on Hermite form of a system and coprime fractions. This technique is implemented in MATLAB and compared to other traditional techniques in terms of three different aspects: The configuration of the realization, memory space and time complexity of the algorithm.

Karim Cherifi
institute of electrical and electronic engineering (ex INELEC) Boumerdes Algeria.
cherifikarimdz@gmail.com

Kamel Hariche
University of Boumerdes
khariche@yahoo.com

CP2

Hamilton-Jacobi Equations in High Dimensions and Its Application to a Class of Optimal Control Problems

In this talk we present some results about target tracking and Hamilton-Jacobi equations. We make some connections between a class of standard optimal control problems with target tracking problems. We develop some numerical methods based on Hamilton-Jacobi equations that allows us to perform computations in high dimensions. We present some numerical results.

Taewoo Kim
Division of Applied Mathematics, Brown University
taewoo_kim@brown.edu

CP2

Preconditioned Warm-started Newton-Krylov Methods for MPC with Discontinuous Control

We present Newton-Krylov methods for efficient numerical solution of optimal control problems arising in model predictive control, where the optimal control is discontinuous. As in our earlier work, preconditioned GMRES practically results in an optimal $O(N)$ complexity, where N is a discrete horizon length. Effects of a warm-start, shifting along the predictive horizon, are numerically investigated. The method is tested on a classical double integrator example of a minimum-time problem with a known bang-bang optimal control.

Andrew Knyazev
Mitsubishi Electric Research Laboratories (MERL)
knyazev@merl.com

Alexander Malyshev
Univ. of Bergen, Norway
alexander.malyshev@uib.no

CP2

Efficient Time Domain Decomposition Algorithms for Time-dependent PDE-constrained Optimization Problems

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, while, with the cost of solving a large scale, fully discrete optimality system. Hence, such one-shot method 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 its 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.

Jun Liu
Jackson State University
jun.liu@jsums.edu

Zhu Wang
Department of Mathematics
University of South Carolina
wangzhu@math.sc.edu

CP2

An Iterative Method for Optimal Control of Pa-

rameterized Bilinear Systems

Optimal control of bilinear systems has been a well-studied subject in the areas of mathematical and computational optimal control. However, effective methods for solving emerging optimal control problems involving an ensemble of deterministic or stochastic bilinear systems are under-developed. These burgeoning problems arise in diverse applications from quantum control and molecular imaging to neuroscience. In this work, we develop an iterative method to find optimal controls for an inhomogeneous bilinear ensemble system with free-endpoint or fixed-endpoint conditions. The central idea is to represent the bilinear ensemble system at each iteration as a time-varying linear ensemble system, and then solve it in an iterative manner. We analyze convergence of the iterative procedure and discuss optimality of the convergent solutions. The method is directly applicable to solve the same class of optimal control problems involving a stochastic bilinear ensemble system driven by independent additive noise processes. We demonstrate the robustness and applicability of the developed iterative method through practical control designs in neuroscience and quantum control.

Jr-Shin Li, Shuo Wang
Washington University in St. Louis
jsli@wustl.edu, swang35@wustl.edu

CP3

Real-time Control for the Stabilization of a Double Inverted Pendulum

We present the real-time implementation of two control strategies to balance a double inverted pendulum (DIP) on a cart. The DIP is considered to be stabilized when the two pendulums are aligned in a vertical position. The mathematical model for the dynamics of the DIP is derived using the Lagrange's energy method which is computed from the calculation of the total potential and kinetic energies of the system. This results in a highly nonlinear system of three second order ordinary differential equations. For our first control, we linearize the system around its zero equilibrium state and implement a linear quadratic regulator (LQR)-based controller to stabilize the system in real-time. Then we implement a controller based on the power series expansion of the Hamilton Jacobi Bellman (HJB) equation. Both simulation and real-time experimental results are presented.

Amanda Bernstein
North Carolina State University
ascoons@ncsu.edu

Hien Tran
Center for Research in Scientific Computation
North Carolina State University
tran@ncsu.edu

CP3

Approximation of Lyapunov Functions from Noisy Data

Methods have previously been developed for the approximation of Lyapunov functions using radial basis functions. However these methods assume that the evolution equations are known. We consider the problem of approximating a given Lyapunov function using radial basis functions where the evolution equations are not known, but we instead have sampled data which is contaminated with noise.

We propose an algorithm in which we first approximate the underlying vector field, and use this approximation to then approximate the Lyapunov function. Our approach combines elements of machine learning/statistical learning theory with the existing theory of Lyapunov function approximation. Error estimates are provided for our algorithm. This is joint work with Peter Giesl, Martin Rasmussen and Kevin N. Webster

Peter Giesl
University of Sussex
p.a.giesl@sussex.ac.uk

Boumediene Hamzi
Koc University
Department of Mathematics
boumediene.hamzi@gmail.com

Martin Rasmussen
Imperial College London
m.rasmussen@imperial.ac.uk

Kevin Webster
knwebster@gmail.com
imperial college london

CP3

On the Stability and the Optimal Decay in a Viscoelastic Problem

In this talk we discuss the following viscoelastic equation $u_t t - ?u + ?_0^t g(t - t?)?u(.,t)dt = 0$, in a bounded domain $?ofR^n(n=1)$ with a smooth boundary, where the relaxation function g is positive nonincreasing and satisfying $g'(t) = -?(t)g^p(t)$, for $? : R^+?R^+$, a decreasing function and $1 = p < 3/2$. We establish a new general decay rate for the solution energy. This work answers some questions raised in the literature and generalizes and improves some earlier results.

Salim Messaoudi
KFUPM, Dhahran, Saudi Arabia-31261
Messaoudi@kfupm.edu.sa

Waled Al-Khulaifi
KFUPM
alkhulaifi@kfupm.edu.sa

CP3

Control of Support Structure Motions of Guyed Offshore Wind Turbines under Environmental Disturbances

Offshore wind turbines supported on guyed towers are inherently complex and respond nonlinearly under wind and wave loading. The motions on the top of the towers structure may be considerably high in severe environmental conditions and therefore they need to be controlled for operational as well as maintenance. Moreover as they are exposed to combined wind and wave loading and are themselves mechanisms, therefore they manifest chaotic behaviour owing to the parametric nonlinearities The undesired chaotic motions are eliminated using the geometrical control methods and thereby the behaviour is synchronized. A 5MW NREL wind turbine is considered for the study. The focus of this paper is to develop a robust control technique so as to regulate the vibration and synchronization of support structures for an offshore wind

turbine. The work is restricted to understanding the non-linear motions of guyed platforms, due to slackening of a guylines and thereby controlling the motions for safe operations. The restoring force of the multiple guylines is idealized as a nonlinear spring whose stiffness changes depending on the position of the structure. In particular, a control mechanism based on backstepping method is being proposed. The performance of the algorithm is illustrated in this paper by designing the controllers for controlled response of the structures supporting guyed wind turbines in the chaotic regime which can be modelled as a Duffing-van-der-Pol oscillator.

Manikandan Rajasekaran
Research Scholar, Department of Ocean Engineering ,
Indian Institute of Technology
mkaucbe@gmail.com

CP3
Control and Stabilization of the Periodic Fifth Order Korteweg-De Vries Equation

We establish local exact control and local exponential stability for fifth order Korteweg-de Vries type equations in $H^s(\mathbb{T})$, $s > 2$. A dissipative term is incorporated into the control which, along with a propagation of regularity property, yields a smoothing effect that permits the application of a contraction principle argument.

Derek Smith
École Polytechnique Fédérale de Lausanne
derek.smith@epfl.ch

Cynthia Flores
California State University
Channel Islands
cynthia.flores@csuci.edu

CP4
Liability and Dividend Management for Insurance Companies

We will consider asset and liability management of insurance companies that choose reinsurance tools to hedge risks. The insurer is risk averse and aims to maximize the expected total discounted value of the utility of dividends paid out under the liability management constraint. Using dynamic programming principles, optimal liability ratio and dividend payment strategies are studied in various cases. Explicit solutions of optimal strategies are obtained in special cases.

Zhuo Jin
The University of Melbourne
zhuo.jin@unimelb.edu.au

CP4
A Market Driver Volatility Model via Policy Improvement Algorithm

In the over-the-counter market in derivatives, we sometimes see large numbers of traders taking the same position and risk. When there is this kind of concentration in the market, the position impacts the pricings of all other derivatives and changes the behaviour of the underlying volatility in a nonlinear way. We model this effect using Heston's stochastic volatility model modified to take into account the impact. The impact can be incorporated into the model using a special product called a market driver, potentially with a large face value, affecting the underlying volatility itself. We derive a revised version of Heston's partial differential equation which is to be satisfied by arbitrary derivatives products in the market. This enables us to obtain valuations that reflect the actual market and helps traders identify the risks and hold appropriate assets to correctly hedge against the impact of the market driver. Furthermore, we use the Policy Improvement Algorithm to optimally approximate our nonlinear partial differential equation (PDE) via series of linear PDEs. The optimal choice of control in each step in the algorithm allows us to obtain the approximated solutions that show quadratic local convergence to the original analytic solution.

Jun Maeda
University of Warwick
J.Maeda@warwick.ac.uk

Saul Jacka
Statistics Dept, University of Warwick
s.d.jacka@warwick.ac.uk

CP4
An Optimal Consumption Problem For a Stochastic Hybrid Model With Delay

In real life, investors tend to look at the historical performance of the risky assets while they are making their investment decisions. In other words, for a more efficient model , memory has to be represented in the dynamics of the process. For this purpose, we extend the Stochastic Maximum Principle for a Markov Regime Switching Jump-Diffusion model with delay. We establish necessary and sufficient maximum principle for such a system. We show that corresponding adjoint equations are given by Anticipated Backward Stochastic Differential Equations and prove the existence-uniqueness theorem for these equations. We illustrate our results by a problem of optimal consumption problem from a cash flow with delay and regimes.

Emel Savku, Gerhard Wilhelm Weber
Middle East Technical University
Institute of Applied Mathematics
esavku@gmail.com, gweber@metu.edu.tr

CP4
A Markov-driven Portfolio Execution Strategy Across Multiple Venues with Market Impact

We propose a framework for studying optimal execution strategies in a limit order book (LOB). The market depth of the LOB is modeled by a finite-state continuous-time Markov chain, and the dynamics of the stock mid-price is modeled by the Markov-modulated Almgren-Chriss market impact model. We consider an agent who seeks to execute a large portfolio using limit and market orders across multiple venues under daily liquidity constraints. Due to insufficient liquidity, an immediate execution is often not possible or at a vey high cost. A slowly liquidation process, however, is often costly, since it may involve undesirable price movements. In this paper, we approach the optimal execution problem from the standpoint of a risk-nuetral agent with the aim of maximizing the expected net financial returns. We obtain our results using the stochastic control approach and develop a suboptimal execution strategy to control the overall tradeoff between liquidation costs and the overnight risk, during which no trade is allowed. Although the strategy we obtain is not the optimal,

it provides better returns for the same risk when compared with the Almgren-Chriss strategy where only market orders are used.

Qingqing Yang
University of Hong Kong
kerryyang920910@gmail.com

CP4

A Constrained Stochastic Control Problem with Application to an Illiquid Stock Position Build-up

We consider a class of constrained stochastic optimal control problems with applications to an illiquid stock position build-up. Using a geometric Brownian motion model, we allow the drift to be purchase-rate dependent to characterize "price impact" of heavy share accumulation over time. The constraint is the fund availability. That is, the expected fund availability has an upper bound. We use a Lagrange multiplier method to treat the constrained control problem. Because a closed-form solution is virtually impossible to obtained, we develop approximation schemes, which consist of inner and outer approximations. The inner approximation is a numerical procedure for obtaining optimal strategies based on a fixed parameter of the Lagrange multiplier. The outer approximation is a stochastic approximation algorithm for obtaining the optimal Lagrange multiplier. Convergence analysis together with numerical examples are provided.

Xianggang Lu
Sun Yat-Sen University
sysuxiangganglu@gmail.com.

George Yin
Wayne State University
gyin@math.wayne.edu.

Qing Zhang
The University of Georgia
qz@uga.edu.

Caojin Zhang
Wayne State University
fl4390@wayne.edu

Xianping Guo
Sun Yat-Sen University
mcsgxp@mail.sysu.edu.cn.

CP5

Modeling the Impact of Climatic Variables on Malaria Transmission

Malaria is one of the most severe disease in the world. The projected climate change will probably alter the region and transmission potential of malaria in Africa. In this study, a climate-based mathematical model to investigate the impact of temperature and rainfall on malaria transmission is developed and analysed. The basic reproduction number $(R\ 0\ )$ is derived along with stability analysis. The effect of the larval death rate on the reproduction number is also investigated. The model is validated on observed malaria transmission in Limpopo Province, South Africa, giving a reasonable fit and in particular, detecting accurately all the spikes in malaria prevalence. The model provides a numerical basis for further refinement towards prediction of the impact of climate variability on malaria transmission.

Gbenga J. Abiodun
University of the Western Cape
3109433@myuwc.ac.za

CP5

Simultaneous Null Controllability of Nonlinear Parabolic Equations

This paper is concerned with a null controllability problem for nonlinear parabolic equations appearing in mathematical biology. We consider a system of two equations with a nonlocal nonlinearity, in a bounded domain Ω of $\mathbb{R}^{N_0}$, N_0 being a positive integer sufficiently small. An operator is nonlocal in the sense that one needs the value of a function in all Ω to determine the effect of the operator on it, and not only in a neighbourhood of a point. Such models can be used in the context of dynamics of biological systems to describe the migration of population (of bacteria in a container). They can also describe the distribution of heat in a conductor. Our aim is to find a control common to both nonlinear equations, which solves the null controllabillity of the studied system under constraints on the state. A similar control problem has recently been addressed for the laplacian operator, so the present paper extends those results. Our work is organized as follows. First, we linearize the studied system in two phases. As a first step we use the Taylor formula, and in a second step we introduce a function fixed in $(L^2(\Omega \times (0,T)))^2$, $T > 0$, in place of the nonlinearity. Under suitable assumptions on the coefficients, this thorough linearization brings back to a null controllability problem with constraints on the control and the latter was solved before. Finally we achieve the result using the Schauder Fixed-point Theorem.

Carole Louis-Rose
Université des Antilles
carole.louis-rose@univ-antilles.fr

CP5

Mathematical Modeling and Quantitative Analysis of Obesity-related Dynamic Scheme for African Americans

Rates of overweight and obesity have increased across the United States among people of all ethnic and racial groups, all ages and both genders, but some groups are disproportionately affected. Among U.S. adults, Black and Latino populations have substantially higher rates of obesity than do White populations. This is true among both men and women. I will summarize the different obesity models that have been published or presented at international conferences. I limit the models that incorporate trends in obesity over time with transitions by ethnic and racial groups, explains how models are constructed, shows the utility of Mathematical Models, and discusses their strength and weakness.

Xiuquan Wang
Tougaloo College
xiuquan0418@gmail.com

CP6

Error Bounds on the Solution to an Optimal Control Problem over Clustered Consensus Networks

In this paper, we obtain a bound on the error term of the solution to a control constrained, linear-quadratic optimal

control problem over a clustered consensus network. For large scale systems, the solution may be regarded as computationally infeasible due to the increase in dimensionality. However, the two time-scale property of the network that arises from the cluster formation indicates that the optimal control problem can be written in standard singularly perturbed form. Thus, we are able to obtain a reduced dimension optimal control problem over a reduced dimension network where individual nodes within a cluster are collapsed into an aggregate node. The solution to the reduced problem can be shown to be asymptotically equivalent in the singular perturbation parameter δ to the solution of the original problem. However, for many values of δ this asymptotic result may fail to be of practical use. We improve on this result by applying a duality theory to the clustered network and derive an upper bound $\chi_u(\delta)$ and lower bound $\chi_l(\delta)$ on the solution to the optimal control problem that holds for arbitrary δ and, furthermore, satisfies the inequality $|\chi_u(\delta) - \chi_l(\delta)| = O(\delta)$ as $\delta \to 0$.

Sei Howe
Imperial College London
sei.howe11@imperial.ac.uk

CP6

Synchronization Conditions for Nonhomogenous Kuramoto Oscillators using Power Series Methods

The well-known Kuramoto model is widely used to study the synchronization in a network of coupled oscillators in many various discipline including biology, physics, social networks, and smart grids. For a nonhomogenous Kuramoto model the problem of phase synchronization of oscillators has been completely addressed in the literature. However, except for some specific networks, the characterization of the frequency synchronization of nonhomogenous Kuramoto oscillators is far from complete. In this talk, we first review the connection between the frequency synchronization of coupled oscillators and existence of an equilibrium point for the Kuramoto map in a specific domain. This connection enables us to focus on the algebraic solutions of the Kuramoto map. Then, using different tools from theory of several complex variables, we derive the power series expansion for the inverse Kuramoto map. We will show that, by truncating this power series, one can get a family of sufficient conditions as well as a family of approximate conditions for frequency synchronization of nonhomogenous Kuramoto oscillators. One of the nice features of these families of conditions is that by increasing the number of terms in truncations, they approach to a necessary and sufficient condition.

Saber Jafarpour
University of California Santa Barbara
saber.jafarpour@engineering.ucsb.edu

Francesco Bullo
Mechanical Engineering
University of California at Santa Barbara
bullo@engineering.ucsb.edu

CP6

Green's Function Approach for Approximate Controllability of Linear Systems

A mathematical approach for finding control functions, providing the required state of a *linear* system in given finite time, is suggested. Representing the solution of the governing initial-boundary value problem in terms of

Green's function and satisfying the desired conditions, a system of equality type constraints on the control function is derived. Solving those constraints together with compatibility constraints of the problem, the control function is found explicitly (non-uniquely).

Asatur Khurshudyan
Institute of Mechanics
National Academy of Sciences of Armenia
khurshudyan@mechins.sci.am

Ara Avetisyan
Institute of Mechanics
National Academy of Armenia
ara.serg.avetisyan@gmail.com

CP6

Prediction of Traffic Jams over Road Networks

Cascading effect of events is a common phenomena observed in network systems. Typical scenarios include propagation of faults in power networks or spread of infectious diseases. In this work, we model propagation of traffic congestion on a given stretch of road starting from a junction with traffic signals. We assume that all the vehicles are homogeneous, with identical dynamics. We develop a deterministic model inspired by the susceptible-infected-susceptible (SIS) model of virus propagation combined with fluid-based traffic models. We call vehicles infected if they face the same red light (stop) signal more than once, which may lead to congestion over some portion of the road stretch under consideration. The congestion reaches a traffic jam/epidemic threshold if the congestion area and the traffic density are above certain critical values. The model captures the transient and asymptotic behaviours of the traffic congestion over time. We present conditions leading to two limiting situations: (i) quick dissipation of congestion and (ii) congestion leading to a traffic jam. The model can also predict if the vehicles are prone to get stuck in congestion and the waiting times of vehicles with respect to their positions on the road. Further, we study the propagation of congestion on the given road, to the network of roads in a region with their own individual traffic conditions modelled in the same way as stated above. We corroborate our models with simulation studies.

Surya Prakash Malladi, Subhadeep Kumar, Ramkrishna Pasumarthy, Nirav Bhatt
IIT Madras
mvsuryaprakash@gmail.com,
kr.subhadeepkumar@gmail.com,   ramkrishna@ee.iitm.ac.in, niravbhatt@iitm.ac.in

CP6

Heuristic Approach to the Efficient Control of Complex Networks

The ability to control natural or technological systems depends on our understanding of the fundamental laws that govern their behavior. Recent research has applied control theory to classify large systems modeled as networks of communicating components based on their controllability, i.e. whether it is possible at all to control them, and if so, the cost of such control in terms of number of driver nodes that must be used to bring them to the desired state, and the number of steps required to do so among other metrics. Algorithms have been developed to identify minimal sets of driver nodes when they exist. Complex systems mod-

eled as complex networks exhibit emergent behavior that is hard or prohibitive to predict, analyze, and control. Even when theoretically feasible, analytical approaches are not computationally prohibitive. On the other hand, in many applications, it is not necessary for a control to be full or optimal to be useful. We develop a cost effective heuristic approach to controlling a system by seeking a tradeoff between the amount of work required to design the control, the percentage of the network controlled, and the cost of exercising the control. Using simulation to create networks of different sizes and topologies, we establish cost spectra that allow users to select the tradeoff that meets their application needs. The heuristic approach builds on prior theoretical and experimental results. It is tested and validated using randomly generated networks.

Babak Ravandi, Forough Sheikh Ansari, Fatma Mili
Purdue University
bravandi@purdue.edu, f.sheikhansari@gmail.com, mili@purdue.edu

CP6
Analyzing Controllability of Bilinear Systems via Symmetric Groups

Bilinear systems emerge in a wide variety of fields as natural models for dynamical systems ranging from robotics to quantum dots. Analyzing controllability of such systems is of fundamental and practical importance, for example, for the design of optimal control laws, stabilization of unstable systems, and minimal realization of input-output relations. Tools from Lie theory have been adopted to establish controllability conditions for bilinear systems, and the most notable development was the Lie algebra rank condition (LARC) which, however, may be computationally expensive for high-dimensional systems. In this work, we present an alternative and effective algebraic approach to investigate controllability of bilinear systems. The central idea is to map Lie bracket operations of the vector fields governing the system to permutation multiplications in a symmetric group, so that controllability and controllable submanifolds can be characterized by permutation cycles. The method is further applicable to characterize controllability of systems defined on undirected graphs, such as multi-agent systems with controlled couplings between agents and Markov chains with controlled transition rates between states, and, consequently, reveals a representation of controllability through connected graphs.

Jr-Shin Li, Wei Zhang
Washington University in St. Louis
jsli@wustl.edu, wei.zhang@wustl.edu

CP7
Information-theoretic Data Association over Nonuniform Partitions

Information theoretic measures of data association allow many-many relationships to be quantified. This is essential since the dimensionality of the phenomenon to be modeled is often not conformal with the dimensionality of the measurement space. In these cases projections lead to confusion when using measures of central tendency in the identification of the mapping domain. The problem is especially egregious in mid to high dimensionality cases where local optimization techniques fail due to sparsity of data supporting local functional estimates. In previous work, parsimonious maps were demonstrated between discrete domain and target random variables by the maximization of mu-

tual information over probability estimates derived from uniform partitions of the spaces under a fixed penalty for partition entropy. In this work we loosen the mapping constraints by allowing for nonuniform partitions determined under several formulations of the partition entropy penalty. In doing so we determine an equivalence between the codebook entropy of the partition construction and the reduction of mapping entropy under the maximization of mutual information between domain and target spaces. Results are shown for several standard data mining datasets.

Paul Deignan
L-3 Communications / IS
Paul.Deignan@utdallas.edu

CP7
Investigating Periodic Attractors of Wind Turbine's Dynamics with Pitch Activated under Control Limits

In this paper we investigate whether continuous oscillations are probable for the wind turbines dynamics when connected to the grid. This can have negative consequences on the power grid and possibly on other power systems connected to the same grid. We consider the wind turbine when the pitch control is activated, exposing it to higher wind speeds. In order to find out if there are continuous oscillations in the state variables that may realistically occur, we investigate if there are periodic attractors for the dynamics that are still allowed within the control limits suggested by many in the literature, such as General Electric. The paper provides rigorous mathematical proofs for boundedness of the systems state variables and their derivatives under the control limits. This establishes the existence of attractors in a bounded system under the control. We then find that there is a Hopf bifurcation in which periodic attractors within the control limits exist. The results are supported by simulations.

Sameh Eisa
New Mexico Tech
sameh.eisa@student.nmt.edu

CP7
Real-time Control Analysis of a 3D Self-balancing Inverted Pendulum and Cart System for Stability in the Event of a Sensor Failure

This paper documents the study of a two-wheeled robotic chassis that successfully and consistently self-balances. Previous approaches to similar models have derived their dynamics from first principles using Newtonian mechanics for a linearized, shared-axle system and Lagrangian mechanics for a linearized, independently-actuated system. This project specifically focuses on a more complicated system with independently-actuated wheels, for which a sophisticated and realistic dynamic model is derived using non-linear Lagrangian mechanics. The pendulum and cart movements are each assumed to be planar, and their planes of motion are defined perpendicular to each other. The systems performance is analyzed in MATLAB to determine the effect of various controllers and filters on stability in cases of full and partial state feedback with and without sensor noise. Performance is characterized in terms of pendulum angle relative to the vertical axis and cart trajectory relative to the ground plane, both of which are functions of the voltage-applied force on each wheel independently. A comparison of the simulations results shows that the non-linear Lagrangian model best fits the true data and yields

less uncertainty given a sensor failure. Based on the deterministic parameters of this model, a recommendation is made about which combination of controllers and filters best maintains the systems stability in the event of a sensor failure returning only partial state feedback.

Sarah T. Lamb, Patricia Mellodge, Kiwon Sohn, Akin Tatoglu
University of Hartford
slamb@hartford.edu, mellodge@hartford.edu, sohn@hartford.edu, tatoglu@hartford.edu

CP7
Optimal Motion Planning to Control Ensemble Properties of Robot Swarms

In large robot swarms, planning individual trajectories compatible with a mission or specified collective purpose can be challenging and computationally intensive. The mission, however, may often be translated into requirements for certain time-dependent ensemble properties of the swarm, without the need to prescribe the exact trajectory of each robot. In these cases, the motion-planning problem can be solved in the low-dimensional space of the ensemble property of interest, and the solution lifted to the full configuration space to generate robot trajectories. Here we focus on the ensemble inertia tensor, which captures the second moment of the spatial distribution of robots in the swarm. We exploit a novel fibering of configuration space (*ensemble fibering*) and the Ehresmann connection associated to kinetic energy, to lift trajectories in the space of inertia tensors to trajectories for the robot swarm. In particular, we derive the optimal robot trajectories to achieve a desired ensemble inertia tensor in finite time, by lifting path-energy minimizing geodesics connecting the initial inertia tensor of the swarm to the desired one. These trajectories can be trivially modified to simultaneously achieve a desired position for the centroid of the swarm. Motion planning in this style is computationally efficient, as its complexity does not grow with the number of robots, and it enables control of the position and spatial extent of the swarm in each direction.

Matteo Mischiati
HHMI Janelia Research Campus
mischiatim@janelia.hhmi.org

CP7
Parameter Estimation and Model Discrimination of Batch Solid-liquid Reactors

Estimation and inference in nonlinear dynamic systems are of significant importance in many practical applications, especially in industrial process systems. However, obtainable measurements are usually limited without enough information for determining an over-parameterized process model. Motivated by this, a procedure of parameter estimation is explored and implemented to pre-select estimable parameter sets, determine parameter values and analyze estimation results. The optimization-based estimation is carried out simultaneously with data reconciliation using the errors-in-variables-measured (EVM) formulation, followed by post-optimality evaluations. Finally, posterior model identification is performed to discriminate multiple potential models and select the most likely one. The proposed estimation procedure is applied on a heterogeneous solid-liquid batch reactor, based on a real-world process with industrial data. Limitations include an unknown reaction mechanism, and that most states cannot be measured directly. By our estimation strategy, inestimable parameters are eliminated and model simplified. Results show good fitting on process data and small variances, which indicates good model parameter selection and estimation. The estimated model is further validated by a new batch of data and k-fold cross validation. These results lead us to elucidate the likely mechanistic model for subsequent optimization studies.

Yajun Wang
Carnegie Mellon University
yajunwan@andrew.cmu.edu

Mukund Patel, Yisu Nie, John Wassick
The Dow Chemical Company
mrpatel@dow.com, ynie@dow.com, jmwassick@dow.com

Lorenz T. Biegler
Carnegie Mellon University
Pittsburgh, USA
biegler@cmu.edu

CP8
Further Remarks on Input-output Linearization of Siso Time-varying Delay Systems

In this paper, the problem of input-output linearization of nonlinear single-input single-output time-varying delay systems (with delays in the input and the output) is discussed and illustrated via several examples. Sufficient conditions for existence of a coordinate change and a nonlinear feedback that linearizes the input-output behavior and stabilizes such systems, have been recently developed by the authors. Here, we propose to discuss these conditions and give some insight allowing to improve these conditions.

Ihab Haidar
Supélec-CNRS-Univ Paris Sud
ihab.haidar@lss.supelec.fr

Florentina Nicolau
INSA Rouen
florentina.nicolau@insa-rouen.fr

Woihida Aggoune
ENSEA
aggoune@ensea.fr

Jean-Pierre Barbot
ECS-Lab, EA 3649
ENSEA
barbot@ensea.fr

CP8
Robust Image Transmission Scheme Based on Coupled Fractional-order Chaotic Maps

In this paper, we propose a novel image transmission scheme based on fractional-order discrete-time systems and on observers design. At the transmitter level, a grayscale original image is encrypted using chaotic signals generated from two different fractional-order chaotic systems. These signals should be available at the receiver level in order to recover this image at the reception end. This is why, two fractional-order observers are used to estimate the states of each fractional-order systems. In addition, in order to show the effectiveness of the proposed transmission system, simulation results will be illustrated and different analysis

is given to illustrate and highlight the security and robustness of the proposed scheme.

Jean-Pierre Barbot
ECS-Lab, EA 3649
ENSEA
barbot@ensea.fr

Ouerdia Megherbi
L2CSP, University of Mouloud Mammeri, Tizi-Ouzou
meg_ouer@yahoo.fr

Sarah Kassim, Saïd Djennoune
L2CSP, University of Mouloud Mammeri, Tizi-Ouzou,
Algeria
kassim.sarah91@gmail.com, s_djennoune@yahoo.fr

Maamar Bettayeb
University of Sharjah
maamar@sharjah.ac.ae

CP8

Fractional Nonlinear Output Error System Identification

This paper deals with identification of fractional nonlinear systems. Hammerstein models are considered, they present unknown inner variables in the information vector. To overcome this difficulty, an identification scheme can be derived based on an auxiliary model which allows to replace the unknown variable with the output of the auxiliary model. An output error method combined with the auxiliary model is used to identify the fractional Hammerstein system. Various simulations test the efficiency of the algorithm in the presence of white output noise.

Karima Hammar, Tounsia Djamah
University M. Mammeri of Tizi Ouzou
kari_auto@yahoo.fr, djamaht_ummto@yahoo.fr

Maamar Bettayeb
University of Sharjah
maamar@sharjah.ac.ae

CP8

The Unicycle in Presence of a Single Disturbance: Observability Properties

This paper investigates the observability properties of a mobile robot that moves on a planar surface by satisfying the unicycle dynamics and that is equipped with exteroceptive sensors (visual or range sensors). In accordance with the unicycle dynamics, the motion is powered by two independent controls, which are the linear and the angular speed, respectively. We assume that both these speeds are known. We consider the case when the robot motion is affected by a disturbance (or unknown input) that produces an additional (unknown and time dependent) robot speed along a fixed direction. The goal of the paper is to obtain the observability properties of the state that characterizes the robot configuration. The novelty of this observability analysis is that it takes into account the presence of an unknown and time dependent disturbance. Previous works that analyzed similar localization problems, either did not consider the presence of disturbances, or assumed disturbances constant in time. In order to deal with an unknown and time dependent disturbance, the paper adopts and improves a new analytic tool, able to solve the nonlinear unknown input observability problem in the case of a single unknown input and various known inputs. We show that the application of this analytic tool is very simple and can be implemented automatically.

Agostino Martinelli
INRIA
agostino.martinelli@inria.fr

CP8

Estimation and Identification for Wireless Sensor Network undergoing Uncertain Jumps

Network control systems are usually modeled as simple channels having limited transmission bandwidth, nonnegligible communication delays and random packet dropouts, when contaminated by disturbances with Gaussian distributions. However, wireless sensor networks undergo several abrupt jumps that appear as discontinuities that can be modeled as non-Gaussian processes, for which the estimation and identification problem is challenging. We consider a stochastic state space model in which the signal is disturbed with Levy-type processes. An approximated ensemble Kalman filter is proposed and a method for the sequential importance sampling is given in the signal estimation stage. Comparison between two filtering methods is investigated, which then leads us to a study of particle MCMC method that is adjusted to achieve the model parameter identification.

Xiaoyang Pan
University of Tennessee
pan@math.utk.edu

Seddik Djouadi
Department of Electrical Engineering and Computer
Science
University of Tenneessee, Knoxville
djouadi@eecs.utk.edu

MS1

Control of Transport PDE/Nonlinear ODE Cascades with State-dependent Propagation Speed

In this paper, we deal with the control of a transport PDE/nonlinear ODE cascade system in which the transport coefficient depends on the ODE state. We develop a PDE-based predictor-feedback boundary control law, which compensates the transport dynamics of the actuator and guarantees global asymptotic stability of the closed-loop system. The stability proof is based on an infinite-dimensional backstepping transformation and a Lyapunov-like argument. The relation of the PDE-ODE cascade with a state-dependent propagation speed to an ODE system with a state-dependent input delay, which is defined implicitly via an integral of past values of the ODE state, is also highlighted and the corresponding equivalent predictor-feedback design is presented together with an alternative proof of global asymptotic stability of the closed-loop system based on the construction of a Lyapunov functional. The practical relevance of our control framework is illustrated in an example that is concerned with the control of a metal rolling process.

Mamadou L. Diagne
Department of Mechanical, Aerospace, and Nuclear
Engineering
Rensselaer Polytechnic Institute
controlatdiagne@gmail.com

Nikolaos Bekiaris-Liberis
Technical University of Crete
Greece
nikos.bekiaris@dssl.tuc.gr

Andreas Otto
Institute of Physics
Chemnitz University of technology
andreas.otto@physik.tu-chemnitz.de

Miroslav Krstic
University of California, San Diego
Dept of Mechanical & Aerospace Engineering
krstic@ucsd.edu

MS1

Stability Analysis of the Fourth-order ODE Analogous to a Piezoelectric Beam PDE

Stability analysis is conducted for a nonlinear fourth-order ordinary differential equation (ODE). The motivation for considering this finite-dimensional equation comes from the initial-boundary-value problem of a piezoelectric beam. In the linearization, stretching and bending are decoupled. This implies that the bending cannot be stabilized by the applied voltage. However, in the original PDE, these equations are coupled. The stability of a related ODE is considered here. This ODE shares a similar structure with the PDE; in particular, has similar time evolution of the PDE although of course neglects the spatial variation within the PDE. Thus, this research can be considered as a preliminary effort for stability analysis of the piezoelectric beam. A novel Lyapunov functional is constructed, based on which the ODE is proved to be locally asymptotically stable around the origin, with a polynomial decay rate. This approach could hopefully give some insights onto the original PDE problem.

Shuxia Tang
Department of Mechanical and Aerospace Engineering
University of California San Diego
shuxiatang.control@gmail.com

Kirsten Morris
Dept. of Applied Mathematics
University of Waterloo
kmorris@uwaterloo.ca

Jean-Michel Coron
Université Pierre et Marie Curie, France
coron@ann.jussieu.fr

MS1

Exact Controllability for Nonlinear Monodomain Equations

In this paper local exact controllability to the trajectories for the one-dimensional monodomain equations with the FitzHugh-Nagumo and Rogers-McCulloch ionic models using distributed controls with a moving support is investigated. In a first step a new Carleman inequality for the linearized monodomain equations, under assumptions on the movement of the control region is presented. It leads to null controllability at any positive time. Subsequently, a local result concerning the exact controllability to the trajectories for the nonlinear monodomain equations

is deduced.

Karl Kunisch
Karl-Franzens University Graz
Institute of Mathematics and Scientific Computing
karl.kunisch@uni-graz.at

Diego Souza
Department of Mathematics and Statistics
Federal University of Pernambuco, Brazil
diego.souza@dmat.ufpe.br

MS1

Persistence Criteria for the Nonlocal Niche Model and Applications

Long range dispersal is a common phenomenon in biology and ecology. To have a better understanding of the evolution of biodiversity in some ecosystem, there is a need to understand the influence of nonlocal dispersals on the survival/persistence of a population. In this talk, I will report on a recent study concerning persistence criteria in some nonlocal models on temporal and spatial heterogeneous environment. I will first present some spectral theory of the associated eigenvalue problem, such as the existence of the principal eigenvalue, and the asymptotic behaviors of the generalized principal eigenvalue with respect to its underlying parameters. As a consequence, I will discuss the applications of these results to the evolutionary invasion analysis. Secondly, I will show some results of the eigenvalue problem with indefinite weight functions, which have practical importance in the context of reserve design or pest control.

Wenxian Shen
Auburn University
wenxish@mail.auburn.edu

Xiaoxia Xie
Department of Mathematics and Statistics
Idaho State University
xiexia2@isu.edu

MS2

An Efficient Algorithm That is Suitable for Embedded Systems for Solving a Class of Optimal Control Problems in High Dimensions

We present some efficient algorithms for solving a large class of optimal controls in high dimensions based on Hamilton-Jacobi equations. The main idea relies on using some representation formulas for the solution of some Hamilton-Jacobi equations. These representation formulas involves convex optimization problems which can be numerically and efficiently solved on embedded systems.

Jerome Darbon
Brown University
jerome_darbon@brown.edu

MS2

Some Examples of Causality-free Algorithms

If a computational algorithm for PDEs can find the value of the solution at a given point without using the value of the solution at any nearby points in the state space, the algorithm is said to be causality free. Two examples are presented using causality free methods. The first example

is a 6D HJB equation for the optimal control of rigid bodies. In this example, the causality free algorithm is applied to sparse grids. The computation at grid points is perfectly parallel. In the second example, we solve a conservation law with a convex flux. In this example, we explore the connections between the entropy solution of scalar convex conservation laws and optimal control theory as well as the associated Pontryagins minimum principle, which leads to a causality free numerical method. The algorithm does not need a grid. The error does not propagate in space. As a result, the algorithm can be used to solve problems having a large number of shocks and still achieve high accuracy around the shocks.

Wei Kang
Naval Postgraduate School
Department of Applied Mathematics
wkang@nps.edu

Lucas Wilcox
Department of Applied Mathematics
Naval Postgraduate School
lwilcox@nps.edu

MS2
Overcoming the Curse of Dimensionality for Hamilton-Jacobi Equations with Applications to Control and Differential Games

In a sequence of papers we developed very fast (e.g $10^{(-7)}$) seconds per evaluation, and embarrassingly parallel methods to solve initial value problems for Hamilton-Jacobi (HJ) equations in a high number of space dimensions. This began with HJ equations depending only on grad(u) arising in control theory, then included differential games, then problems with linear controls and now, it appears, we can also do this for nonconvex Hamiltonian which are state (x) dependent. The idea is to generalize the Hopf-Lax formulas and to solve the resulting optimization problems using techniques involving the level set method and familiar splitting techniques, arising, e.g., in compressed sensing.

Stanley J. Osher
University of California
Department of Mathematics
sjo@math.ucla.edu

Jerome Darbon
Brown University
jerome_darbon@brown.edu

Ya-Tin Chow
UCLA
ytchow@math.ucla.edu

MS2
Computational Challenges in the Numerical Approximation of Nonlinear Functionals and Functional Differential Equations

In this talk we address a rather neglected but very important research area in computational mathematics, namely the numerical approximation of nonlinear functionals and functional differential equations (FDEs). FDEs are of fundamental importance in many areas of mathematical physics, such as fluid dynamics (Hopf characteristic functional equation of turbulence), statistical physics (effective action methods), quantum field theory (Schwinger-Dyson equations), and control theory. However, no effective numerical method has yet been developed to compute effectively their solution. In this talk, I will provide a new perspective on this general problem, and discuss recent progresses in approximation theory for nonlinear functionals and FDEs. The proposed new methods will be demonstrated in various examples.

Daniele Venturi
Department of Applied Mathematics and Statistics
University of California Santa Cruz
venturi@ucsc.edu

MS3
Reaction Diffusion Equations and their Optimal Control with Potential Application to Biomedical Problems

In this talk we consider control problems for a class of reaction diffusion equations with polynomial nonlinearities. We prove existence of mild solutions under the assumption that the nonlinear term is strongly coercive. Next we relax this assumption and consider the natural state space for diffusions and prove existence of mild solutions locally. Using these existence results we formulate some optimal control problems and prove existence of optimal controls. Following this we develop necessary conditions of optimality. Then we consider a class of population problems, as special case of the general reaction diffusion equations, and apply the optimal control theory to immunotherapy whereby physicians can determine the optimal strategy for drug administration to cancer patients.

Nasir Ahmed
Faculty of Engineering
University of Ottawa
ahmed@eecs.uottawa.ca

MS3
Infinite-dimensional Pontryagin Principles for Systems Discrete-time Infinite-horizon Optimal Control Problems

We present new statements of Pontryagin principles for discrete-time infinite-horizon optimal control problems when the state space and the control space are infinite dimensional. In comparison with existing results on this question, we avoid to use several assumptions on the finiteness of the dimension (or the codimension) of certain subspaces.

Joël Blot
University Paris 1
joel.blot@univ-paris1.fr

MS3
The HJB-POD Approach for Infinite Dimensional Control Problems

We propose a computational approach for the solution of an optimal control problem governed by evolutive PDEs equation. Our aim is to obtain approximate feedback laws by means of the application of the dynamic programming principle. Since this methodology can be applied only to low-dimensional dynamical systems, we first introduce a reduced-order model for the dynamics by means of Proper Orthogonal Decomposition. The coupling between the reduced-order model and the related dynamic programming equation allows to obtain the desired approximation of the feedback law. We discuss numerical aspects of this

approach, a-priori error estimates and some applications to parabolic and hyperbolic problems. Works in collaboration with A. Alla (Florida State University), D. Kalise (RICAM) and S. Volkwein (Konstanz).

Maurizio Falcone
Università di Roma "La Sapienza', Italy
falcone@mat.uniroma1.it

MS4

Methods for Robust Control and Performance Analysis via Information Divergences

The goal of robust control is the construction of controls that have provable performance guarantees over specified classes of uncertainties. At the same time, it is important that any approach be computationally tractable. We present an approach possessing both these properties that is based on variational relations between classes of performance measures and corresponding divergences between probability measures (e.g., relative entropy, Rnyi divergence).

Amarjit Budhiraja
Department of Statistics and Operations Research
University of North Carolina at Chapel Hill
budhiraj@email.unc.edu

MS4

Exploiting Low-rank Structure in Stochastic Optimal Control and Filtering Problems

Computational algorithms for stochastic optimal control and estimation quickly encounter the curse of dimensionality–their computational expense grows exponentially with the number of states of the dynamical system. As a result, most algorithms rely on linearizations or control-affine structure of stochastic dynamical systems and therefore generate non-optimal controllers or inaccurate filters. In this talk, we demonstrate how low-rank functional decompositions can enable accurate, real-time control and estimation for general nonlinear stochastic dynamical systems. We use our recently developed function-train decomposition to exploit low-rank structure in both cost functions and differential equations to achieve computational complexity that is linear with dimension and polynomial with function rank. Our control algorithms are demonstrated on a real-time agile robotic system whose goal is to fly quickly though a small window. Our results indicate 5 orders of magnitude reduction in storage cost and computation time as compared to traditional dynamic programming approaches. Finally, we demonstrate applications in estimation with an approach to scale integration-based Gaussian filtering to tens of dimensions while maintaining stability for chaotic systems.

Alex A. Gorodetsky
Massachussets Institute of Technology
goroda@mit.edu

MS4

Sequential Optimal Experimental Design via Stochastic Control

The optimal design for a sequence of experiments in the presence of uncertainty can be formulated as a discrete-time stochastic optimal control problem. Such a formulation accounts for feedback between experiments and for the future consequences of design decisions; this is in contrast to common suboptimal design practices such as open-loop design (choose all experiments simultaneously) and greedy/myopic design (optimally select the next experiment without accounting for future effects). This stochastic control problem is then solved using finite-horizon dynamic programming, maximizing the expected information gain in continuous parameters given continuous design variables and observations. We find near-optimal policies via approximate value iteration. To make this iteration tractable, transport maps are employed to represent non-Gaussian posteriors and to enable fast approximate Bayesian inference. We construct a Knothe-Rosenblatt map that couples a standard Gaussian to the joint distribution of designs, observations, and parameters, where posteriors can be obtained easily by conditioning. Maps are built using trajectories from exploration and exploitation in an adaptive manner, iteratively discovering and increasing accuracy over state regions that are more likely to be visited. The overall method is demonstrated on a problem of optimal sequential sensing: inferring contaminant source location from a mobile sensor in a time-dependent convection-diffusion system.

Xun Huan
Sandia National Laboratories
xhuan@sandia.gov

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS4

Data-driven Reduced-order Models for Control of PDEs with Uncertain Parameters

We present work on data-driven surrogate modeling for online control of complex systems modeled through parameter dependent PDEs. Complex systems in form of PDEs are challenging for model-based feedback control and observer design, since the state space high dimensional. Moreover, the physical parameters of the system are often subject to various uncertainties, adding more complexity to the control problem. We present a data-driven reduced-order modeling framework, which allows us to update reduced-order models with real system data to account for parametric changes online. These updated models can then be used to compute a suboptimal feedback control law. Numerical test problems in form of fluid-dynamical applications are presented.

Boris Kramer
Massachusetts Institute of Technology
bokramer@mit.edu

B. Peherstorfer
University of Wisconsin-Madison
peherstorfer@wisc.edu

Karen E. Willcox
Massachusetts Institute of Technology
kwillcox@MIT.EDU

MS5

Parabolic Equations with Quadratic Growth in R^n

We study here quasi linear parabolic equations with quadratic growth in R^n. These equations are at the core of the theory of P.D.E., see Ladyenskaya et al. and Fried-

man. However, for the applications to physics and mechanics, one deals mostly with boundary value problems. The boundary is often taken to be bounded and the solution is bounded. This brings an important simplification. On the other hand, Stochastic Control leads mostly to problems in R^n. Moreover, the functions are unbounded and the Hamiltonian may have quadratic growth. There may be conflicts, which prevent solutions to exist. In Stochastic Control, a very important development deals with BSDE, (Backward stochastic differential equations). There is a huge interaction with parabolic P.D.E. in R^n. This is why, although we do not deal with BSDE in this paper, we use many ideas from P. Briand, Y. Hu, F. Da Lio, O. Ley, M. Kobylanski, N. El Karoui, S. Hamadene, A. Matoussi. Our presentation is slightly innovative.

Alain Bensoussan
The University of Texas at Dallas and
City University of Hong Kong, Hong Kong
axb046100@utdallas.edu

MS5
On Adaptive Robust Control in Discrete Time

We will present an approach to stochastic control in discrete time subject to model uncertainty. The true model is assumed to belong to a class of models that are parameterized in terms of a finite dimensional parameter. The true parameter is unknown. The controller combines robust optimization and learning using adaptive robust control methodology. The learning amounts to deriving confidence regions for the unknown parameter. The confidence regions are computed on-line, that is recursively. This allows for solving the underlying uncertain stochastic control problem via what we call the adaptive robust dynamic programming. An illustrating example will be presented.

Tomasz Bielecki
Department of Applied Math, IIT
tbielecki@iit.edu

Tao Chen, Igor Cialenco
Illinois Institute of Technology
tchen29@iit.edu, cialenco@iit.edu

Areski Cousin
ISFA Actuarial School
University of Lyon
areski.cousin@univ-lyon1.fr

Monique Jeanblanc
Université d'Evry Val d'Essonne, France
Monique.Jeanblanc@univ-evry.fr

MS5
Approximations for Average Markov Decision Processes in Continuous-time

This talk is concerned with numerical methods for solving continuous-time Markov decision processes. We are interested in approximating numerically the value function of a general controlled model $\mathcal{M}$ with Borel state and action spaces, under the expected long run average cost optimality criterion. Our approach, loosely speaking, consists in approximating a set of two optimality inequalities for the model $\mathcal{M}$ by means of a discretization of the state and action spaces of $\mathcal{M}$. To do so, we assume that the positive part of the transition rate governing the dynamics of the control model $\mathcal{M}$ has a density function with respect to a reference probability measure μ. It will be shown that the error between the optimal values of $\mathcal{M}$ and $\mathcal{M}_{k,\delta}$ can be controlled through the values of the Wasserstein distance $\mathcal{W}(\mu, \mu_k)$ between μ and μ_k and the Hausdorff distance between $\mathbf{A}(x)$ and $\mathbf{A}_\delta(x)$. We study also the particular case when empirical probability measures are used to approximate the reference probability measure μ and show that convergence of the approximation takes place at an exponential rate in probability.

Jonatha Anselmi
INRIA Bordeaux Sud-Ouest
jonatha.anselmi@inria.fr

Francois Dufour
Institut de Mathematiques de Bordeaux
Universite Bordeaux 1
francois.dufour@math.u-bordeaux.fr

Tomas Prieto-Rumeau
Statistics Dept, UNED
tprieto@ccia.uned.es

MS5
Regime-Switching Jump Diffusions: Coupling Method, Feller and Strong Feller Properties

This work focuses on a class of regime-switching jump diffusion processes, in which the switching component has countably infinite many states or regimes. The existence and uniqueness of the underlying process are obtained by an interlacing procedure. Then the Feller and strong Feller properties of such processes are derived by the coupling method and an appropriate Radon-Nikodym derivative. Finally the paper studies exponential ergodicity of regime-switching jump-diffusion processes.

Fubao Xi
Beijing Institute of Technology
xifb@bit.edu.cn

Chao Zhu
University of Wisconsin-Milwaukee
zhu@uwm.edu

MS6
A General Valuation Framework for Sabr and Stochastic Local Volatility Models

In this talk, we propose a general framework for the valuation of options in stochastic local volatility (SLV) models with a general correlation structure, which includes the Stochastic Alpha Beta Rho (SABR) model as a special case. Standard stochastic volatility models, such as Heston, Hull-White, Scott, Stein-Stein, α-Hypergeometric, $3/2$, $4/2$, mean-reverting, and Jacobi stochastic volatility models, also fall within this general framework. We propose a novel double-layer continuous-time Markov chain (CTMC) approximation respectively for the variance process and the underlying asset price process. The resulting regime-switching continuous-time Markov chain is further reduced to a single CTMC on an enlarged state space. Closed-form matrix expressions for European options are derived. We also propose a recursive risk-neutral valuation technique for pricing discretely monitored path-dependent options, and use it to price American, and barrier options. In addition, we provide *single* Laplace transform formulae for arithmetic Asian options as well as occupation time derivatives. Numerical examples demonstrate the accu-

racy and efficiency of the method using several popular SLV models, and reference prices are provided for SABR, Heston-SABR, quadratic SLV, and the Jacobi model.

Duy Nguyen
Department of mathematics
Marist College
NDUCDUY@GMAIL.COM

MS6

Optimal Oil Production and Taxation in Presence of Global Disruptions

This paper studies the optimal extraction policy of an oil field as well as the efficient taxation of the revenues generated in light of various economic restrictions and constraints. Taking into account the fact that the oil price in worldwide commodity markets fluctuates randomly following global and seasonal macroeconomic parameters, we model the evolution of the oil price as a mean reverting regime-switching jump diffusion process. Moreover, taking into account the fact that oil producing countries rely on oil sale revenues as well as taxes levied on oil companies for a good portion of the revenue side of their budgets, we formulate this problem as a differential game where the two players are the mining company whose aim is to maximize the revenues generated from its extracting activities and the government agency in charge of regulating and taxing natural resources. We prove the existence of a Nash equilibrium and characterize the value functions of this stochastic differential game as the unique viscosity solutions of the corresponding Hamilton Jacobi Isaacs equations. Furthermore, optimal extraction and fiscal policies that should be applied when the equilibrium is reached are derived. A numerical example is presented to illustrate these results.

Moustapha Pemy
Towson University
Department of Mathematics
mpemy@towson.edu

MS6

Valuing Stock Loans using a Markov Chain Model

Two classical mathematical tools used to model stock price movements are Brownian motions and binomial trees. Brownian motions offer nice mathematical properties but only yield closed form solutions in limited situations. On the other hand, binomial trees can be used to price a wide variety of stock market derivatives, but they are difficult to work with mathematically. Markov chain models combine the discrete movements of a binomial tree model while retaining the Markovian properties of Brownian motion, thus allowing the best properties of both of these models. In this talk, we consider a Markov chain model in which the price of the underlying asset is determined by a two-state Markov chain. Such a Markov chain model is strikingly simple and yet captures a wide variety of market movements. By proper selection of parameters, the Markov chain model can produce sample paths that are very similar to or very different from a classical Brownian motion. This talk presents formulas for stock loan valuation, or the value of a loan in which a risky share of stock is used as collateral, under such a model. Dynamic programming equations in terms of variational inequalities are used to capture the problem's dynamics. These equations are solved in closed-form, and explicit optimal solutions are obtained. Numerical examples are also reported to illus-

trate the results.

David J. Prager
Anderson University
dprager@andersonuniversity.edu

Qing Zhang
University of Georgia
qz@uga.edu

MS6

Robust Dynkin Game

We analyze a robust version of the Dynkin game over a set $\mathcal{P}$ of mutually singular probabilities. We first prove that conservative player's lower and upper value coincide (Let us denote the value by V). Such a result connects the robust Dynkin game with second-order doubly reflected backward stochastic differential equations. Also, we show that the value process V is a submartingale under an appropriately defined nonlinear expectations up to the first time τ_* when V meets the lower payoff process. If the probability set $\mathcal{P}$ is weakly compact, one can even find an optimal triple for the value V_0. This is a joint work with Erhan Bayraktar.

Song Yao
University of Pittsburgh
songyao@pitt.edu

Erhan Bayraktar
University of Michigan
Department of Mathematics
erhan@umich.edu

MS7

Control in Structural Brain Networks: Developmental Phenotypes and Rewiring Mechanisms

The human brain is a complex organ characterized by heterogeneous patterns of interconnections. New non-invasive imaging techniques now allow for these patterns to be carefully and comprehensively mapped in individual humans, paving the way for a better understanding of how wiring supports our thought processes. While a large body of work now focuses on descriptive statistics to characterize these wiring patterns, a critical open question lies in how the organization of these networks constrains the potential repertoire of brain dynamics. In this talk, I will describe an approach for understanding how perturbations to brain dynamics propagate through complex writing patterns, driving the brain into new states of activity. Drawing on a range of disciplinary tools from graph theory to network control theory and optimization I will identify control points in brain networks, characterize trajectories of brain activity states following perturbation to those points, and propose a mechanism for how network control evolves in our brains as we grow from children into adults. Finally, I will describe how these computational tools and approaches can be used to better understand how the brain controls its own dynamics (and we in turn control our own behavior), but also how we can inform stimulation devices to control abnormal brain dynamics, for example in patients with severe epilepsy.

Danielle S. Bassett
School of Engineering and Applied Science
University of Pennsylvania

dsb@seas.upenn.edu

MS7

Artificial Control of Real Muscle: FES for Clinical Applications and Movement Science

We control the movements of our body and limbs through our muscles. However, the forces produced by our muscles depend unpredictably on the commands sent to them. This uncertainty has two sources: irreducible noise in the motor system's processes (i.e. motor noise) and variability in the relationship between muscle commands and muscle outputs (i.e. model uncertainty). Any controller, neural or artificial, benefits from estimating these uncertainties when choosing commands. To examine these benefits we developed an in vivo functional electric stimulation (FES) platform for the rat hindlimb, to measure isometric forces. We began by validating the platform, demonstrating our ability to differentially stimulate and control the activation of many muscles. Then we compared an FES controller that represents and compensates for uncertainty in muscle forces, with a standard FES controller that neglects uncertainty. Accounting for uncertainty substantially increased the precision of force control. Our work demonstrates the theoretical and practical benefits of representing muscle uncertainty when computing muscle commands. The findings are relevant beyond FES as they highlight the benefits of estimating statistical properties of muscles for both artificial controllers and the nervous system.

Max Berniker
University of Illinois, Chicago
Department of Mechanical & Industrial Engineering
mbernike@uic.edu

MS7

Adaptive Algorithms for Suppression of Neural Biomarkers with Deep Brain Stimulation

Deep brain stimulation is used for treating Parkinsons disease, essential tremor, and epilepsy, and there is interest in using it for many other neurological diseases. Deep brain stimulation devices have many parameters, such as voltage and stimulation frequency, that can be adjusted by the clinician. Adjusting the parameters is a lengthy and somewhat haphazard process. New devices allow us to monitor neural activity from deep brain stimulation leads not being used for stimulation (Stypulkowski, 2014). This provides us with the opportunity to use machine-learning algorithms to optimize stimulation parameters based on biomarkers. For suppression of seizures we have developed a closed-loop stimulation using a Linear Quadratic Regulator that reduces spontaneous epileptiform neural activity in vivo. For Parkinson's disease we have developed a reinforcement learning algorithm to discover a stimulation policy based on phase and amplitude of beta oscillations to maximally suppress the pathological neural activity.

Theoden I. Netoff
University of Minnesota
Department of Biomedical Engineering
tnetoff@umn.edu

Vivek Nagaraj, Logan Grado
University of Minnesota
Dept. of Biomedical Engineering

nagar030@umn.edu, grado@umn.edu

MS7

Open Versus Closed Loop Control in a Respiratory Model

Incorporation of sensory feedback is essential to guide the timing of rhythmic motor processes. How sensory information influences the dynamics of a central pattern generating circuit varies from system to system, and general principles for understanding this aspect of rhythmic motor control are lacking. It has been realized for sometime, however, that the mechanism underlying rhythm generation in a central circuit when considered in isolation may be different from the mechanism underlying rhythmicity in the intact organism [Bassler, Biol Cybern 54:65-69, 1986]. We analyze open-loop versus closed-loop control of a respiratory control system incorporating a central pattern generator (the Butera-Rinzel-Smith neuron model [Butera et al., J Neurophys. 82:382-397, 1999]), motor output driving gas exchange in the lung, transport of oxygen from the lung to the bloodstream, and chemosensory feedback from hypoxia sensors in the carotid body to an excitatory tonic conductance in the BRS model neuron. Surprisingly, during normal, eupneic breathing, the feedback control signal lies in a range for which a steady state analysis predicts quiescence of the CPG, rather than steady bursting. In addition, we show that conductances endogenous to the BRS model of the respiratory CPG can lead to spontaneous autoresuscitation after short or mild bouts of hypoxia, and we analyze the system dynamics at the boundary separating eupnea from tachypnea, or pathologically rapid, shallow breathing.

Casey Diekman
Department of Mathematical Sciences
New Jersey Institute of Technology
casey.o.diekman@njit.edu

Peter J. Thomas
Case Western Reserve University
pjthomas@case.edu

Chris Wilson
Loma Linda University
School of Medicine
cgwilson@llu.edu

MS8

Smarter Grids using Distributed Learning Control

The emerging science of smart grids has often featured people from outside the area of power grids who are not engaged with the needs of industry and often ignore the existing science of power grids built up for nearly a century. The lead author has been participating in moves (see Power Globe for instance) towards a revival of a more considered scientific approach such as happened in the power grids area from the late 70's to the mid 90's (and led to many of the leaders of fundamentals of power grids such as Ilic, Wu, Sauer etc). The lead author is a long-standing participant in the study of power grids with a strongly scientific view (he is also independently active in stability theory, control theory and network science) and the other coauthors are younger experts in control theory and learning respectively. This paper will review some recent progress with a more scientific view to complement and enhance the

more realistic developments in industry.

David Hill, Tao Liu, Haomin Ma
The University of Hong Kong
dhill@eee.hku.hk, taoliu@eee.hku.hk, hmma@eee.hku.hk

MS8
Smart Grid in a Room Simulator (SGRS): A Tool for Assessing Effects of Smarts in Electric Energy Systems

As new technologies get integrated into the existing electric energy systems it is critical to design cyber (control, communications) for enabling their desired performance. For example, it is hard to integrate large amount of solar or wind power without creating operating problems such as instabilities, or even lack of feasible equilibrium. We briefly summarize fundamental roadblocks to doing this using best industry practices of today. We next show how a carefully designed simulation platform can be used to benchmark dynamic response of changing electric power grids with various embedded cyber (control, communications). We describe how one such general simulation platform, known as SGRS, is designed using automated modeling of these systems in standard state space form. This simulator is particulary focused on the ability toshow effects fo embedded control. We illustrate the modeling approach and use of SGRS on two real-world local electric power grids by emulating dynamic response of these grids. This is done to demonstrate the effects of best industry practices and to compare them with performance of the same grids with several newly proposed control methods for microgrids.

Marija Ilic, Rupamathi Jaddivada
Carnegie Mellon University
milic@ece.cmu.edu, rjaddiva@mit.edu

MS8
Coalitional Games and Grid Integration of Renewable Energy

In this presentation, we will showcase a collection of results that employ ideas, frameworks, techniques, and results from the field of coalitional game theory to address some key issues in grid integration of renewable electricity generation. Inherent uncertainty and uncontrollability of wind and solar electric energy production poses significant challenges in integrating these generation resources into electric power systems. Aggregation over diverse geographical locations can be a powerful approach to reduce the impact of uncertainty and variability. Coalitional games provide an excellent framework for analyzing and designing appropriate schemes to take advantage of aggregation. Aggregation costs and benefits need to be allocated participating entities. It is necessary to ensure that such allocations are fair and lead to desirable (stabilizing) behaviors by the participants. We will discuss some recent results on the problem of causation based allocation of costs and benefits that arises in electric power systems.

Pramod Khargonekar
University of California, Irvine
pramod.khargonekar@uci.edu

P. Chakraborty
University of California, Berkley
prats19@gmail.com

E. Baeyens

University of Valladolid, Spain
enrbae@eis.uva.es

MS8
Distributed Optimal Power and Voltage Management in DC Microgrids

This paper develops new control strategies to address fundamental issues of power balance, line loss reduction, and voltage profile management in DC microgrids. In microgrids of distributed renewable generations and controllable loads, load allocation to different distributed generators, line losses, voltage stability and quality are intimately coupled, departing significantly from traditional power grids in which economic dispatch and voltage stability are typically separate control and management issues. In this paper, a multi-objective optimization strategy is introduced to address such a challenge. The competing objectives of feeder current balance power loss reduction, and voltage deviation attenuation are expressed in a global optimization index. The corresponding global optimal solutions are derived. To reduce operational costs, improve robustness and reliability, and provide scalability, local recursive optimization algorithms for distributed control strategies are sought, in the framework of weighted and constrained consensus. While in most application problems, distributed optimization methods can only achieve suboptimal solutions due to limitations on their information structures, this paper shows that by designing suitable local optimization criteria and recursive algorithms, our local recursive consensus-type algorithms are convergent to the global optima. Case studies using DC-powered trolleybus systems are conducted to evaluate the algorithms.

Eyad Sindi, Le Yi Wang
Wayne State University
eyad.sindi@wayne.edu, lywang@ece.eng.wayne.edu

Michael P. Polis
Oakland University
polis@oakland.edu

George Yin
Wayne State University
gyin@math.wayne.edu.

Lei Ding
Swinburne University of Technology
Melburne, Australia
dl522@156.com

MS9
Generalized Characteristics and Singularities of Solutions to Hamilton-Jacobi Equations

For stationary Tonelli Hamiltonians we develop an intrinsic proof of the existence of generalized characteristics using sup-convolutions for the so-called fundamental solution. This approach, together with local convexity estimates for the fundamental solution, leads to a new understanding of the global propagation of singularities and of their connectedness properties.

Piermarco Cannarsa
University of Rome "Tor Vergata"

cannarsa@mat.uniroma2.it

MS9
First and Second Order Necessary Conditions for Stochastic Optimal Controls

Although the stochastic optimal control theory was developing almost simultaneously with the deterministic one, its results are much less fruitful than those obtained for the deterministic control systems. The main reasons are due to some essential difficulties (or new phenomena) when the diffusion term of the stochastic control system depends on the control variable and the control region lacks convexity. We establish the first and second order necessary optimality conditions for stochastic optimal controls using the classical variational analysis approach and the convex duality. The control system is governed by a stochastic differential equation, in which both drift and diffusion terms may contain the control variable and the set of controls is allowed to be nonconvex. The end point constraints are of the inequality type. Only one adjoint equation is introduced to derive the first order necessary optimality condition; while only two adjoint equations are needed to state the second order necessary conditions for stochastic optimal controls. Compared to the existing results obtained by the spike variations, the main advantage of the classical variational analysis approach is due to weaker smoothness requirements imposed on the coefficients of the control system and the cost functional (with respect to the state variable) and to fewer adjoint equations needed to state these conditions.

Helene Frankowska
CNRS and IMJ-PRG UPMC Paris 6
helene.frankowska@imj-prg.fr

Haisen Zhang
Southwest University, Chongqing
China
haisenzhang@yeah.net

Xu Zhang
Sichuan University, Chengdu
China
xuzhang@amss.ac.cn

MS9
Normality of the Pontryagin Maximum Principle for Infinite Dimensional Control Systems under State Constraints

We consider a Mayer problem associated to a semilinear control system of the form

$$\dot{x}(t) = Ax(t) + f(t, x(t), u(t)),$$

with $x(\cdot)$ staying in a given closed subset of an infinite dimensional separable Banach space and $u(\cdot)$ varying in a complete separable metric space. The presence of the operator A, the infinitesimal generator of a strongly continuous semigroup, makes this system a convenient tool for the study of control problems involving PDEs. We provide estimates on the distance of a mild solution of the control system to the set of all solutions lying in the given constraint set. These results can be applied to prove non degenerate necessary optimality conditions. This is a joint work with Hélène Frankowska and Elsa Maria Marchini.

Marco Mazzola

Dept. Mathematics, UPMC, Paris, France
marco.mazzola@imj-prg.fr

MS9
Optimal Control of Hereditary Systems

Time delays are encountered in many areas of control engineering, including process control where they are associated with transport delays of reagents flowing between reactors, and control applications in planetary exploration where communications delays are an important factor. This presentation concerns necessary conditions for optimal control problems involving time delays. Necessary conditions for time delay problems, in the form of a generalized Pontryagin Maximum Principle, go back to the early days of optimal control theory. But a number of important issues have until recently remained unresolved; these concern optimality conditions covering free end-time problems, optimality conditions for problems involving noncommensurate delays in the control, and versions of the necessary conditions which are valid for non-smooth data. We provide an overview of recent developments. Special attention is given to new two-sided necessary conditions for free end-time problems that improve on former one-sided conditions. We explain their relevance to sensitivity analysis and the computation of optimal controls for time delay systems. We focus also on new integral versions of the Weierstrass condition, discuss their significance and illustrate, through examples, respects in which they improve on traditional pointwise versions of the condition.

Richard B. Vinter
Imperial College, Exhibition Road, London SW7 2AZ, UK
r.vinter@imperial.ac.uk

MS10
A Functional Analytic Approach to Approximate Iterative Algorithms

We consider the problem of replacing a fixed point algorithm $V_n = TV_{n-1}$, $n \geq 1$, based on operator T, with an approximate algorithm $V_n = \hat{T}_n V_{n-1}$, where $\hat{T}_n$ defines a sequence of operators approximating T in some sense. The objective is to characterize the convergence of the approximate algorithm to the original fixed point $V^* = TV^*$. A general functional analytic approximation model, defined on a normed vector space, will be described for such algorithms. This model permits generalized definitions of the error tolerance of approximate operators, and establishes continuity relationships between operators and approximate fixed point solutions. In this way, the convergence rates of approximate algorithms can be studied for broad classes of algorithms using essentially one single theory. It will be shown how the theory can be used to determine convergence properties for general classes of algorithms, such a stochastic approximation and fixed point iteration of nonexpansive maps, using only Banach space properties. The theory will also be applied to Markov decision processes, showing how convergence properties of various adaptive value iteration techniques can be deduced and optimized.

Anthony Almudevar
University of Rochester
Dept of Biostatistics and Computational Biology
anthony_almudevar@urmc.rochester.edu

MS10
Clustered Information Filter for Markov Jump Lin-

ear Systems

Minimum mean square error estimation for linear systems with Markov jump parameters is addressed. The jump variable is assumed to be observed, however only cluster information is taken into account in the filter design, allowing one to seek for the best implementable estimator via the cardinality and choice of the clusters. With this new approach we introduce a set of filters that can be compared in terms of performance according to the refines of clusters of the Markov chain. Moreover, it includes as particular cases the well known Kalman filter with as many clusters as Markov states, as well as the linear Markovian estimator with only one cluster. The Riccati-like formulas for pre-computation of gains are given, and we explore the trade-off between complexity and performance via numerical examples.

Eduardo F. Costa
Universidade São Paulo
Instituto de Cincias Matemáticas e de Computação
efcosta@icmc.usp.br

MS10

Stochastic Approach of Fragmentation - Application to Avalanches

The aim of this talk is to introduce a numerical probabilistic approach for an avalanche-type process. The originality of our approach is to use a fragmentation model to describe the avalanche phenomenon. We start by introducing a new interpretation of the fragmentation equation by means of branching processes. A particular fragmentation kernel, which is discontinuous, leads to a stochastic model for the fragmentation phase of an avalanche. For these processes, solutions of some particular stochastic differential equations of fragmentation, we construct a numerical approximation scheme. We analyse in particular this numerical results on our model of avalanches and emphasize the fractal property observed theoretically in our model. This is a joint work with Lucian Beznea (IMAR, Bucharest) and Oana Lupaşcu (IMAR, Bucharest).

Madalina Deaconu
Inria Nancy - Grand Est
IECL
madalina.deaconu@inria.fr

MS10

Optimal Stopping for Change-point Detection of Piecewise Deterministic Markov Processes

We consider a problem of change point detection for a continuous-time stochastic process in the family of piecewise deterministic Markov processes introduced by MHA Davis in the 80's. The process is only observed in discrete time and with noise, and the aim is to accurately detect the (random) time when its dynamics change and also select the new dynamics among a finite number of possibilities as soon as possible after the change-point. To do so, we turn the detection problem into an optimal stopping problem for partially observed Markov decision process with values in a continuous state space, and provide a discretization of the state space to be able to solve the problem numerically. Applications include for instance maintenance optimization where the change-point corresponds to a failure time of some equipment. Another application concerns treatment optimization for cancer patients. The change-point then corresponds to a sudden deterioration of the health of the patient. It must be detected early so that the treatment can be adapted.

Benoite de Saporta
University of Bordeaux
benoite.de-saporta@umontpellier.fr

Alice Cleynen
CNRS - IMAG
alice.cleynen@umontpellier.fr

MS11

Control of Voluntary Immunosuppression in Transplant Patients

When formulating mathematical models to improve our understanding of biological processes, it is not always possible to find all parameter values in literature. In such cases, and in the presence of data, inverse problems are performed to estimate these unknown parameters. Statistical error models used during inverse problem formulations help quantify the uncertainty and variability that arises with using experimental data. There is a relatively recent research effort in modeling the infections related to solid organ transplants. We present mathematical and statistical models for renal transplant recipients infected by BK virus. Using a second order difference-based method to eliminate statistical error model misspecification, we show how modified residuals from the inverse problem can be used to detect discrepancies in mathematical model formulation. The problem of appropriate control of the suppression levels in long term individual patient therapy is addressed.

H.T. Banks
htbanks@ncsu.edu
NC State University

Rebecca A. Everett
Arizona State University
rarodger@asu.edu

Neha Murad
Center for Research in Scientific Computation
North Carolina State University, Raleigh, NC, USA
nmurad@ncsu.edu

MS11

Different Numerical Aspects for Dirichlet Boundary Control Problems

This talk is concerned with error estimates for the solution of finite element discretized linear elliptic equations in weighted L^2-norms containing the distance to the boundary as a weight function. These error estimates are of interest when deriving discretization error estimates for the normal derivative of the solution. As an application, we use this result for the numerical analysis of Dirichlet control problems, where the control variable corresponds to the normal derivative of some adjoint variable. Our aim is to improve the accuracy of the numerical approximation by refining the computational meshes towards the boundary of the underlying domain. More precisely, in the context of Dirichlet control problems, we show that a convergence rate of almost two can be achieved for the discrete optimal controls if the appearing corner singularities are mild enough and if the meshes are sufficiently graded towards the boundary. Finally, the predicted convergence rates are

confirmed by numerical examples.

Johannes Pfefferer
Technische Universität München
Zentrum Mathematik
pfefferer@ma.tum.de

Max Winkler
Universität der Bundeswehr München
max.winkler@unibw.de

MS11
Applications of Nonlocal PDE-constrained Optimization in Economics

In this presentation we consider economic models originally developed by Ramsey to model the financial behavior of households in an economy. The new aspect of our research is the inclusion of a continuity of households which leads to the use of PDEs. In order to incorporate also the effect of agglomeration we formulate the model in terms of nonlocal diffusion processes or partial integro-differential equations. We present result on the theory and numerics of the models and formulate corresponding optimization problems.

Ekkehard W. Sachs, Laura Somorowsky
University of Trier
sachs@uni-trier.de, somorowsky@uni-trier.de

MS11
Modeling and Optimization of a Process of Semiconductor Crystal Growth

We report on the control of the turbulent flow in a semiconductor melt. By a new technology, the melt flow is influenced by traveling magnetic fields that are generated in a so-called heater-magnet module (HMM). The HMM contains the induction coils that generate the heat in the crystal melt and also the Lorentz forces for stirring the melt. The main goal of optimization is the following: In a certain point of the melting pot, the temperature of the melt should oscillate with high frequency but low amplitude. In contrast to former technologies, the HMM is located inside the crucible, and hence the control of the Lorentz forces is much more efficient to meet the objective of optimization than former technologies. In the talk, mathematical models for the control problem are discussed and an associated optimal control problem is set up. Main emphasis is laid on the numerical method for solving the system of state equations that account for heat transport, melt flow, and Lorentz forces. Moreover, we explain the selection of objective functionals for expressing the goal of optimization. Numerical examples are presented.

Olaf Klein
Weierstrass-Institute Berlin
olaf.klein@wias-berlin.de

Peter Nestler, Nico Schlömer
TU Berlin, Institute of Mathematics
nestler.peter@googlemail.com, nico.schloemer@gmail.com

Jürgen Sprekels
Weierstrass-Institute Berlin
sprekels@wias-berlin.de

Fredi Tröltzsch
Techn. University of Berlin
Institute of Mathematics
troeltzsch@math.tu-berlin.de

MS12
Decomposition of Reachable Sets and Tubes for a Class of Nonlinear Systems

Hamilton-Jacobi (HJ) reachability provides formal guarantees for performance and safety properties of nonlinear control systems with bounded disturbances. Here, one aims to exactly compute the backward reachable set (BRS) or tube (BRT) – the set of states from which the system can be driven into a target set at a particular time or within a time interval, respectively. The computational complexity of current approaches scales exponentially, making application to high-dimensional systems intractable. We propose a technique that decomposes the dynamics of a general class of nonlinear systems into subsystems which may be coupled through common states, controls, and disturbances. Despite this coupling, BRSs and BRTs can be computed efficiently and exactly using our technique without the need for linearizing dynamics or approximating sets as polytopes. Computations of BRSs and BRTs now become orders of magnitude faster, and for the first time BRSs and BRTs for many high-dimensional nonlinear control systems can be exactly computed. In situations where the exact solution cannot be computed, our proposed method can obtain slightly conservative results. We demonstrate our theory by numerically computing BRSs and BRTs for several systems, including the 6D Acrobatic Quadrotor and the 10D Near-Hover Quadrotor.

Mo Chen, Sylvia Herbert, Mahesh Vashishtha, Somil Bansal
UC Berkeley
mochen72@berkeley.edu, sylvia.herbert@berkeley.edu, msv@berkeley.edu, somil@berkeley.edu

Claire J. Tomlin
University of California, Berkeley
tomlin@eecs.berkeley.edu

MS12
Pareto Front Characterization for Multi-Objective Optimal Control Problems using HJB Approach

In this work we present a new approach for the characterization of the Pareto front for multi-objective optimal control problems with state constraints. Our approach is based on the HJB (Hamilton-Jacobi-Bellman) theory. A general bi-objective constrained optimal control problem is considered. First, we introduce an auxiliary optimal control problem for an augmented dynamical system. It turns out that the Pareto front for the multi-objective optimal control problem is characterized as a subset of the zero-level set of the value function associated with the auxiliary control problem. This characterization leads to a numerical procedure for computing the Pareto front and the corresponding optimal trajectories from the augmented value function. A Pareto front characterization is also derived in a special case where one of the criteria is a minimum time to reach a target set. Some numerical examples are presented in this work to show the relevance of our approach.

Anna Desilles
ENSTA ParisTech
adesilles@gmail.com

Hasnaa Zidani

ENSTA ParisTech, INRIA Saclay
hasnaa.zidani@ensta-paristech.fr

MS12

Applications of the Generalized Hopf Formula to Linear Control Problems

Traditionally, numerical solutions to Hamilton-Jacobi equations require a dense, discrete grid of the solution space. Computing the elements of this grid scales poorly with dimension and has limited use to problems with dimension of less than four. Recent research has discovered numerical solutions based on the generalized Hopf formula that do not require a grid and can be used to efficiently compute solutions to a certain class of Hamilton Jacobi PDEs that arise in linear control theory and differential games. These new methods were applied to multi-vehicle collaborative pursuit guidance of maneuvering targets. A joint system state space representing the kinematics of all pursuing vehicles relative to the target was constructed, the dimension of which makes it infeasible for traditional grid-based methods. This high-dimensional problem was then efficiently solved using the generalized Hopf formula, and included the constraint of time-varying bounds on the magnitude of available vehicle control, while ensuring intercept when starting within the reachable set. The speed of computation also make these methods attractive for reachability computations to aid reactive, real-time collision avoidance of air vehicles. The aircraft in these systems can have models that easily have state dimension of 12 or more. Reachability is essential for any system to provide provably safe operation, and its application to collision avoidance in dense airspace will be discussed.

Matthew Kirchner
Naval Air Warfare Weapons Division
matthew.kirchner@navy.mil

Gary Hewer
NAWC Weapons Division
Gary.Hewer@navy.mil

Robert Mar, Brian Reitz
Naval Air Warfare Center Weapons Division
robert.t.mar@navy.mil, brian.reitz@navy.mil

Jerome Darbon
UCLA

Stanley J. Osher
University of California
Department of Mathematics
sjo@math.ucla.edu

MS12

Hamilton-Jacobi Equations for Two-Point Boundary-Value Problems in Conservative Systems and Dequantized Schrodinger Equations

Stationary action may be used to address complex-valued dynamical systems. It is also useful in solution of the small-noise limit of dequantized Schrodinger equations. The use of stationary-action to analyze such systems requires an extension of Hamilton-Jacobi theory. Because of the use of stationarity rather than optimization, many classical tools from optimal control theory are inapplicable. Nonetheless, a relation between the viscosity solution of a certain HJ PDE and the associated stationary-action problem may be established. Solutions for complex- and real-valued stationary action problems may be generated from sets of solutions of differential Riccati equations (DREs). Although for optimization problems, one is not interested in propagation of solutions past escape times, this is not the case for problems in stationary action. One method for propagation of the solutions of DREs past escape times is through "static duality". Static duality will be defined, and the use of this tool in propagation of DRE solutions past escape times will be indicated.

William M. McEneaney
Dept. of Mechanical and Aerospace Engineering
University of California, San Diego
wmceneaney@ucsd.edu

Peter M. Dower
The University of Melbourne
pdower@unimelb.edu.au

Ruobing Zhao
Univ. of California San Diego
ruz015@eng.ucsd.edu

MS13

Optimal Control for Pointwise Asymptotic Stability of a Continuum of Equilibria

Pointwise asymptotic stability is a property of the set of equilibria of a dynamical system, where every equilibrium is Lyapunov stable and every solution is convergent to some equilibrium. This property is exhibited, for example, by common convex optimization algorithms in discrete and in continuous time, when minimizers are not unique, and by multiagent systems seeking consensus. Standard Lyapunov conditions are not appropriate for characterization of this property, but set-valued Lyapunov functions are. The talk surveys these topics and then presents how pointwise asymptotic stability can be achieved, in a control system, through open-loop solutions to an infinite-horizon optimal control problem. This applies to continuous time, discrete time, and in fact hybrid which blend continuous and discrete control systems, and in discrete time results in feedback pointwise asymptotic stabilization.

Rafal Goebel
Mathematics and Statistics
Loyola University Chicago
rgoebel1@luc.edu or rafal.k.goebel@gmail.edu

MS13

Exact Test for Real-positiveness of Fractional Systems

We present an algebraic method for testing the real-positiveness of time-invariant fractional linear systems. Our approach relies exclusively on symbolic computations and thus avoids any instability that can appears in numerical algorithms. Moreover we show how our method yields an algorithm to build a feedback that makes the system real-positive. Here again the approach is entirely algebraic and involves only symbolic computations.

Yirmeyahu Kaminski
Department of Applied Mathematics
Holon Institute of Technology

jykaminski@gmail.com

MS13

Optimal Control Problems for a Class of Variational-hemivariational Inequalities with Applications to Elastic Unilateral Frictional Contact

In this talk we study an optimal control problem for a class of nonlinear elliptic variational-hemivariational inequalities. First, for a variational-hemivariational inequality, we prove results on its well posedness and on the approximation of its solution by a sequence of penalized problems. Next, we analyze optimal control problems for both variational-hemivariational inequality and its penalized version. Then, we prove the convergence of the sequence of optimal solutions to control problems for the penalized problem to an optimal solution to the initial variational-hemivariational inequality, when the penalty parameter tends to zero. Finally, we apply the results to a frictional contact problem which describes the contact between an elastic body and the foundation. In this problem the friction law is modeled by a variant of the Coulomb law of dry friction and the multivalued normal compliance contact condition involves unilateral constraints of Signorini type.

Stanislaw Migorski
Faculty of Mathematics and Computer Science
the Jagiellonian University
stanislaw.migorski@gmail.com

MS13

Bolza Optimal Control Problems with Linear Equations and Periodic Convex Integrands on Large Intervals

We study the structure of approximate solutions of Bolza optimal control problems, governed by linear equations, with periodic convex integrands, on large intervals, and show that the turnpike property holds. To have this property means, roughly speaking, that the approximate optimal trajectories are determined mainly by the integrand, and are essentially independent of the choice of time intervals and data, except in regions close to the endpoints of the time interval. We also show the stability of the turnpike phenomenon under small perturbations of integrands and study the structure of approximate optimal trajectories in regions close to the endpoints of the time intervals.

Alexander Zaslavski
The Technion Israel Institute of Technololy
ajzasl@tx.technion.ac.il

MS14

A Locally Adaptive Approach for the Solution of PDEs with Uncertain Inputs

When solving partial di?erential equations (PDEs) with random inputs, it is often computationally ine?cient to merely propagate samples of the input probability law (or an approximation thereof) because the input law may not accurately capture the behavior of critical system responses that depend on the PDE solution. In this work, we develop an adaptive sampling and local reduced basis method for approximately solving PDEs with random inputs. Our method determines a set of parameter atoms and an associated (implicit) Voronoi partition of the parameter domain on which we build local reduced basis approximations of the PDE solution. The atoms are selected in a sequential and adaptive manner using an a posterior error indicator. We pro-vide theoretical error bounds for our approximations and numerically demonstrate the pro?ciency of our method.

Zilong Zou
Duke University
zilong.zoou@duke.edu

Wilkins Aquino
Associate Professor
Dept. of Civil and Environmental Engineering, Duke Univ.
wa20@duke.edu

MS14

Challenges in Discretization of High Dimensional Optimization and Control Problems

In this talk, I will discuss some numerical challenges in dealing with discretization of infinite dimensional optimization and control systems. Examples will be given from projects supported by the DARPA mathematics program.

Fariba Fahroo
DARPA, Defense Sciences Office
fariba.fahroo@darpa.mil

MS14

Optimal Motion Planning with Parameter Dependency

Optimal control problems with parameter dependencies in cost and/or dynamics have arisen in multiple control applications, including ensemble control, optimal search, and robust control. This talk discusses tools for applying computational optimal control techniques to problems with parameter dependencies. These tools include a flexible numerical algorithm for producing solutions using a variety of underlying discretization schemes which can be catered to numerical needs; and analytic conditions for analysis in the form of a Pontryagin-like minimum principle. We apply these to an extended problem formulation for optimal control problems with parameter dependencies which includes multiple types of state, control, and end time constraints.

Qi Gong
University of California, Santa Cruz
qigong@soe.ucsc.edu

MS14

Optimization under Uncertainty of Integrated Circuits

In this talk we discuss simulations and design strategies for integrated circuits (IC) in the presence of uncertainty. We present detailed sensitivity analysis and uncertainty quantification (UQ) simulations for IC on both transistor level and device level, using BSIM model and VTR model. We also discuss the impact of the uncertainties on the design optimization of the ICs.

Dongbin Xiu
Ohio State University

xiu.16@osu.edu

MS15
Rate Control under Heavy Traffic with Strategic Servers

We consider a large queueing system that consists of many strategic servers that are weakly interacting. Each server processes jobs from its unique critically loaded buffer and controls the rate of arrivals and departures associated with its queue to minimize its expected cost. The rates and the cost functions in addition to depending on the control action, can depend, in a symmetric fashion, on the size of the individual queue and the empirical measure of the states of all queues in the system. In order to determine an approximate Nash equilibrium for this finite player game we construct a Lasry-Lions type mean-field game (MFG) for certain reflected diffusions that governs the limiting behavior. Under conditions, we establish the convergence of the Nash-equilibrium value for the finite size queuing system to the value of the MFG. In general closed form solutions of such MFG are not available and thus numerical methods are needed. We use the Markov chain approximation method to construct approximations for the solution of the MFG and establish convergence of the numerical scheme.

Erhan Bayraktar
University of Michigan
Department of Mathematics
erhan@umich.edu

Amarjit Budhiraja
Department of Statistics and Operations Research
University of North Carolina at Chapel Hill
budhiraj@email.unc.edu

Asaf Cohen
University of Michigan
asafc@umich.edu

MS15
Periodic Strategies in Optimal Execution with Multiplicative Price Impact

In this talk we present recent results on the optimal execution problem, when an underlying Poisson process is introduced, representing the opportunities to rebalance the portfolio. This means that when the agent decides to sell some number of shares of the asset at time t, we assume that there is an impact in the price of the risky asset, described as a multiplicative factor. The explicit form of the optimal strategy is provided as well as the form of the value function. This is a joint work with J.L. Perez and Harold Moreno-Franco.

Daniel Hernandez-Hernandez
Centro de Investigacion en Matematicas, Guanajuato, Mexico
dher@cimat.mx

MS15
Pairs-trading under Geometric Brownian Motions

This paper is concerned with an optimal strategy for simultaneously trading of a pair of stocks. The idea of pairs-trading is to monitor their price movements and compare their relative strength over time. A pairs trade is triggered by their prices divergence and consist of a pair of positions to short the strong stock and to long the weak one. Such a strategy bets on the reversal of their price strengths. From the viewpoint of technical tractability, typical pairs trading models usually assume a difference of the stock prices satisfies a mean reversion equation. In this paper, we consider the optimal pairs-trading problem by allowing the stock prices to follow general geometric Brownian motions. The objective is to trade the pairs over time to maximize an overall return with a fixed commission cost for each transaction. The optimal policy is characterized by threshold curves obtained by solving the associated HJB equations. Numerical examples are included to demonstrate the dependence of our trading rules on various parameters and to illustrate how to implement the results in practice.

Qing Zhang
University of Georgia
Department of Mathematics
qingz@math.uga.edu

Jingzhi Tie
University of Georgia
jtie@uga.edu

Hanqin Zhang
National University of Singapore
bizzhq@nus.edu.sg

MS15
Dynamic Convex Duality in Constrained Utility Maximization

We study a constrained utility maximization problem following the convex duality approach. After formulating the primal and dual problems, we construct the necessary and sufficient conditions for both the primal and dual problems in terms of FBSDEs plus additional conditions. Such formulation then allows us to explicitly characterize the primal optimal control as a function of the adjoint process coming from the dual FBSDEs in a dynamic fashion and vice versa. We also find that the optimal primal wealth process coincides with the optimal adjoint process of the dual problem and vice versa. Finally we solve three constrained utility maximization problems and contrast the simplicity of the duality approach we propose with the technical complexity in solving the primal problems directly.

Harry Zheng
Imperial College London
h.zheng@imperial.ac.uk

yusong li
imperial college
y.li11@imperial.ac.uk

MS16
On Mertons Problem with Continuous Wealth Utility

The famous Mertons problem of optimal consumption-investment has a very nice structure which leads to a somewhat explicit solution. The techniques to handle it are for instance to use duality, which linearizes the problem, or to use the so called martingale method. However, this nice mathematical aspects break down, as soon as one introduces a continuous wealth utility term, instead of just the utility of wealth at the horizon. This is a reasonable extension, from the economic standpoint, and a mathematical challenge. In the literature, this extension has been

considered , by trying to generalize the duality approach. Here we use a different technique, which is more straightforward, not relying on duality. This is joint work with Yiqun Li and S.C.P. Yam.

Alain Bensoussan
The University of Texas at Dallas and
City University of Hong Kong, Hong Kong
axb046100@utdallas.edu

MS16

Market-reaction-adjusted Optimal Central Bank Intervention Policy in a Forex Market with Jumps

Impulse control with random reaction periods (ICRRP) is used to derive a country's optimal foreign exchange (ForEX) rate intervention policy when the ForEX market reacts to the interventions. We model the ICRRP problem by using multi-dimensional jump diffusion processes with regime switching. We establish a verification theorem for our control problem, which provides sufficient conditions for the existence of an optimal impulse control with minimum cost. We also use numerical simulation to demonstrate the efficacy of our framework by finding a market-reaction-adjusted optimal central bank intervention (CBI) policy in the ForEX market.

Hongwei Long
Department of Mathematical Sciences
Florida Atlantic University
hlong@fau.edu

MS16

Mean-variance Portfolio Selection for Partially-observed Point Processes

In a ultra-high frequency trading environment, we study the classical meanvariance portfolio selection problem in a partially-observed market with one bond and multiple stocks. Each stock price is modeled as a collection of counting processes, the noisy observation of a intrinsic value process. With incomplete information, we first obtain a separation principle, which involves filtering. Then, we employ stochastic maximum principles for optimal control of forward-backward SDEs with jumps to explicitly derive the efficient strategies. This is joint work with Xiangdong Liu, Jie Xiong, and Shuaiqi Zhang.

Yong Zeng
University of Missouri at Kansas City
Department of Mathematics and Statistics
zengy@umkc.edu

MS16

Optimal Impulse Dividend Control for a Growth-restricted Regime Switching Diffusion

This presentation investigates the impulse dividend optimization problem for a broad class of growth restricted diffusions with drift and volatility dependent on both the level of surplus and the economy regime (described by a Markov chain). There are proportional and fixed costs associated with each dividend payment and the objective of the optimization problem is to maximize expected discounted dividend payments. This work extends Paulsen [Advances in Applied Probability, 39(3):669–689, 2007] by extending the diffusion model to a regime switching diffusion model, and Sotomayor and Cadenillas [Stochastics: An International

Journal of Probability and Stochastic Processes, 85(4):707–722, 2013] by extending the Markov modulated Brownian motion to a much more general class of Markov modulated diffusions. It is shown that for the optimization problem with two regimes, either the optimal strategy is a regime-switching lump sum dividend strategy or there exists no optimal strategy.

Jinxia Zhu
Australian School of Business
The University of New South Wales
Jinxia.zhu@unsw.edu.au

MS17

Controlling Acute Inflammation: A Summary of Strategies

When the natural processes that govern the inflammatory response to severe infection or traumatic insult become dysregulated, intervention is necessary to restore homeostasis to the host. However, knowing how to intervene in order to help guide desirable outcomes is a difficult endeavor due to the complexity of the immune response. Using a canonical and highly nonlinear mathematical model of the systemic acute inflammatory response, we investigate and compare different control strategies to determine therapeutic intervention protocols for a challenging biomedical problem. In particular, we report on results of several methods applied in a diverse virtual patient population with limited measurement feedback. These include nonlinear model predictive control combined with state estimation, optimal control, and a newer method called model free control.

Judy Day, Ouassim Bara
University of Tennessee
judyday@utk.edu, obara@vols.utk.edu

Seddik Djouadi
University of Tennessee at knoxville
Department of Electrical engineering and computer science
mdjouadi@utk.edu

Michel Fliess
LIX (CNRS, UMR 7161) Ecole polytechnique-Paris
ALIEN(Algebre pour Identification & Estimation Numeriques)
michel.fliess@polytechnique.edu

Cedric Join
CRAN (CNRS, UMR 7039), Universite de Lorraine-Nancy
ALIEN(Algebre pour Identification & Estimation Numeriques)
cedric.join@univ-lorraine.fr

Gregory Zitelli
University of California, Irvine
gzitelli@uci.edu

MS17

Optimal Control as a Tool for Designing Better Drug Delivery Schedules

The outcome of drug therapy depends on the combination, concentration, and timing of drug delivery. This is especially true when drugs have differing modes of action

and the underlying network, which describes potential interactions between drugs and the disease state, includes feedback loops. The problem of determining an effective drug delivery schedule can be formulated as an impulse or discrete optimal control problem. In this paper review a method for formulating such a discrete control problem, and discuss the application of this method to a model of cancer cell growth.

Rachel Leander
Middle TN State University
rachel.leander@mtsu.edu

Zack Jones
St. Jude Children's Research Hospital
zack.jones@stjude.org

MS17
Parameter Estimation for Ensemble ODE Models

Ensemble models describe natural phenomena governed by deterministic processes for which the parameters of the system are uncertain, most often due to parameter variability across a spectrum of subjects. This work deals with several aspects of the inverse problem of estimating the parameter density for ordinary differential equation ensemble models from knowledge about data. First, we consider the baseline question of identifiability from a single trajectory in data space, establishing a geometric identifiability condition for linear and linear-in-parameters systems. Next, we derive bounds on how much uncertainty can be tolerated within limited data samples without changing the nature of the inverse problem solution, such as the qualitative properties of the dynamical system corresponding to the inferred parameter values. Finally, we build on these results to relate parameter estimation for ensemble models to Bayesian inference and we show that within this framework, use of an appropriate prior distribution on parameter space is essential to ensure correct results.

David Swigon
Department of Mathematics
University of Pittsburgh
swigon@pitt.edu

Shelby Stanhope
Temple University
stanhope@temple.edu

Jonathan E. Rubin
University of Pittsburgh
Department of Mathematics
jonrubin@pitt.edu

MS17
The Entrain Project: Optimal Control and Circadian Rhythms in the Wild

Circadian clocks govern biological functions that repeat with a period of approximately 24 hours, with light as the primary synchronizer of the human circadian clock. Using techniques from optimal control, we can generate schedules of light and dark that shift a model of the circadian clock to a new time zone as quickly as possible. In April 2014, we released a mobile application, Entrain, for relaying these optimal schedules to travelers crossing multiple time zones. Here I will discuss how the schedules in Entrain are calculated, as well as new approaches that can make the schedules more robust to real world constraints. I will also discuss data collected through Entrain and future directions for the project, including integrating mathematical modeling with wearable devices on mobile platforms.

Olivia Walch
Univeristy of Michigan
ojwalch@umich.edu

MS18
Boundary Observers for Coupled Reaction-diffusion Systems with Applications to Lithium-ion Batteries

We present an observer for a coupled reaction-diffusion PDEs with boundary measurement. We show that, as in the case of stabilization, the backstepping kernel PDEs are essentially equivalent to the PDEs governing the kernels for stabilization of first-order hyperbolic coupled PDEs. The problem we solve is motivated by diffusion phenomena in lithium-ion batteries with electrodes that comprise multiple active materials. Numerical examples are provided for the computation of the kernels.

Leobardo Camacho-Solorio
Department of Mechanical and Aerospace Engineering
University of California, San Diego
lcamacho@eng.ucsd.edu

Rafael Vazquez
Universidad de Sevilla
rvazquez1@us.es

Miroslav Krstic
University of California, San Diego
Dept of Mechanical & Aerospace Engineering
krstic@ucsd.edu

MS18
Life Modeling and Prediction of Large Lithium-ion Battery Packs

Lithium-ion battery (LIB) packs are the most popular chemistry for transportation and stationary energy storage solutions. One challenge in using LIB is to accurately estimate its remaining life. Prognostic life model can be a powerful tool to handle the state of health (SOH) estimate, an enabler for adopting advanced controls in BMS to increase pack utilization, reduce cost, and extend life. The main challenge for SOH estimation is that individual cell ages at various speeds even under same condition due to a number of factors such as the temperature gradient and the quality of manufacturing. When having a large pack with hundreds of cells, the difficulty of estimating pack SOH elevates. This work proposed a life model using both empirical and physical-based approaches. The life model described the compounding effect of different aging on the entire cell with an empirical model. Then its lower-level submodels looked at degradation rates for each aging mechanism. The hybrid approach made the life model generic, robust and stable regardless of battery chemistry and usage. Also, the semi-empirical approach helped to keep the model computationally inexpensive for real-time implementation. Two case studies showed the life model successfully captured the aging trajectories of battery packs under advanced controls.

Ying Shi
Transportation and Hydrogen Systems Center
National Renewable Energy Laboratory

ying.shi@nrel.gov

Kandler Smith
National Renewable Energy Laboratory
kandler.smith@nrel.gov

MS18
State-of-Charge Estimation of Lithium-ion Batteries Modeled by a Coupled PDE-ODE System

A thermal-electrochemical model of lithium-ion batteries is presented, which is a coupled PDE-ODE system, and a backstepping observer is derived for State-of-Charge (SoC) estimation by recovering the lithium concentration in the electrodes. The PDE subsystem is the Single Particle Model (SPM) which is a reduced version of the Doyle-Fuller-Newman (DFN) model for the lithium ion concentration, and the ODE subsystem models the average temperature dynamics. Adding thermal dynamics to SPM serves a two-fold purpose: improving the accuracy of SoC estimation and keeping track of the average temperature which is a critical variable for safety management in lithium-ion batteries.

Shuxia Tang
Department of Mechanical and Aerospace Engineering
University of California San Diego
shuxiatang.control@gmail.com

Leobardo Camacho-Solorio
Department of Mechanical and Aerospace Engineering
University of California, San Diego
lcamacho@eng.ucsd.edu

Yebin Wang
Mitsubishi Electric Research Laboratories
201 Broadway, Cambridge, MA, USA
yebingwang@ieee.org

Miroslav Krstic
University of California, San Diego
Dept of Mechanical & Aerospace Engineering
krstic@ucsd.edu

MS19
Newton-Kantorovich Methods for Nonlinear Constrained Model Predictive Control

A review of Newton-Kantorovich-type computational methods will be presented for both smooth and nonsmooth optimization problems. The methods are applied to model predictive control models based on nonlinear discrete-time optimal control problems with state and control constraints. Advanced-step computational strategies will be discussed. Applications will be presented.

Asen Dontchev
American Mathematical Society
ald@ams.org

MS19
Error Estimates for the Euler Discretization of An Optimal Control Problem with First-order State Constraints

We propose some error estimates for the discrete solution of an optimal control problem with first order state constraints, where the trajectories are approximated with a classical Euler scheme. We obtain order one approximation results in the L^∞ norm (as opposed to the order $2/3$ obtained in the literature). We assume either a strong second order optimality condition, or a weaker formulation in the case where the state constraint is scalar, satisfies some hypotheses for junction points, and the time step is constant. Our technique is based on some homotopy path of discrete optimal control problems that we study using perturbation analysis of nonlinear programming problems.

Adriano Festa
RICAM
Austrian Academy of Sciences
adrianofesta@gmail.com

Frédéric Bonnans
Inria-Saclay and CMAP, Ecole Polytechnique
frederic.bonnans@inria.fr

MS19
Convergence Rate for a Gauss Collocation Method Applied to Constrained Optimal Control

A local convergence rate is established for a Gauss orthogonal collocation method applied to optimal control problems with control constraints. If the Hamiltonian possesses a strong convexity property, then the theory yields convergence for problems whose optimal state and costate possess two square integrable derivatives. The convergence theory is based on a stability result for the sup-norm change in the solution of a variational inequality relative to a 2-norm perturbation, and on a Sobolev space bound for the error in interpolation at the Gauss quadrature points and the additional point -1. A numerical example assesses the limitations of the convergence theory.

William Hager
University of Florida
Department of Mathematics
hager@ufl.edu

Subhashree Mohapatra
Department of Mathematics
University of Florida
subha@ufl.edu

Anil Rao
University of Florida
Mechanical and Aerospace Engineering
anilvrao@gmail.com

MS19
High Order Discrete Approximations to Optimal Control Problems with Bang-bang Solutions

In contrast to optimal problems satisfying strong coercivity conditions, if the optimal control is of bang-bang type the known time-discretization methods ensure at most first order accuracy (with respect to the discretization step) of the approximation to the optimal control. The talk will present a recently developed by the authors approach, which provides accuracy of order $2/\kappa$, where $\kappa \geq 1$ is related to certain controllability properties of the system, and "generically $\kappa = 1$, thus the accuracy is of second order. The approach is based on the Voltera-Fliess (instead of Taylor) series for the differential equation. The discrete-time problem involves control variables that correspond to the zeroth and the first integral moments of the continuous-time control (so the dimension of the control doubles). Al-

though the discrete-time problem is non-coercive, as well, the control set there turns out to be strongly convex, which plays a regularizing role. A procedure for construction of continuous-time controls from discrete-time ones complements the discretization algorithm. The error estimates are obtained by using recent results about metric sub-regularity of the system of necessary conditions of the continuous-time problem. The theoretical results are supported by numerous numerical tests that clearly show the advantage of the new approach.

Teresa Scarinci, <u>Vladimir Veliov</u>
Vienna University of Technology
teresa.scarinci@tuwien.ac.at,
vladimir.veliov@tuwien.ac.at

MS20

Risk-averse Control of Continuous-time Markov Chains

We present time-consistent risk-averse control of continuous-time Markov systems. The approach is based on the dual representation of coherent risk measures, differentiability concepts for set-valued mappings, and a concept of strong time consistency. We use the recent concept of a controlled risk multikernel of a Markov system, which we view as a multifunction and consider its semi-derivatives. We call those derivatives a multi-generator: a concept generalizing the notion of a generator of a Markov process. We derive a system of ordinary differential equations for the new continuous time risk measure. The equations generalize the classical backward Kolmogorov equations for Markov processes. We use them for a risk-averse optimal control problem formulation and derive optimality conditions for it. We construct convergent discrete-time approximations to the continuous-time control problem.

<u>Darinka Dentcheva</u>
Department of Mathematical Sciences
Stevens Institute of Technology
darinka.dentcheva@stevens.edu

MS20

Risk-averse Control of Discrete-time Processes

We discuss risk-averse models of control of discrete-time Markov systems. By using a refined version of time-consistency, we derive the structure of risk measures for such processes, which allows us to represent risk via a composition of a family of so-called transition risk mappings, which evaluate risk of a function of the next process state, given the current transition kernel. This allows for the derivation of dynamic programming equations in finite and infinite time, with or without discount. Special attention will be paid to partially observable models, where the conditional distributions of the unobserved part of the constitute part of the extended state of the system. We derive special structure of transition risk mappings in this case. Finally, we apply our results to the problem of risk-averse optimization of clinical trials. This is joint research with Ozlem Cavus, Jingnan Fan, and Curtis McGinity.

<u>Andrzej Ruszczynski</u>
Rutgers University
rusz@business.rutgers.edu

MS20

Risk Models for Partially Observable Continuous-time Markov Systems

We provide a theory of time-consistent dynamic risk measures for partially observable Markov jump process in continuous time. By introducing risk filtering, which is a new 2-stage risk measure, we show that the risk measure of a partially observable system can be represented as a risk measure of a fully observable system that is defined by g-evaluation. The innovation process of the original system is the Brownian Motion driving the new fully observable system. Furthermore, we introduce a risk-averse control problem for the partially observable system and weak formulation is established for the purpose of risk-averse dynamic programming equation. Finally, we prove that the value function of the risk-averse control problem is a viscosity solution of a special Hamilton-Jacobi-Bellman equation. We also prove a verification theorem.

<u>Ruofan Yan</u>
Department of Mathematics
Rutgers University
ry91@math.rutgers.edu

MS20

Numerical Methods of Risk-averse Control of Diffusion Processes

We propose a numerical recipe for risk evaluation defined by a backward stochastic differential equation. Using dual representation of the risk measure, we convert the risk valuation to a stochastic control problem where the control is a certain Radon-Nikodym derivative process. By exploring the maximum principle, we show that a piecewise-constant dual control provides a good approximation on a short interval. A dynamic programming algorithm extends the approximation to a finite time horizon. Finally, we illustrate the application of the procedure to risk management in conjunction with nested simulation.

<u>Jianing Yao</u>
Royal Bank of Canada
New York
yaojn_1@hotmail.com

MS21

Constrained Optimization for Identification of PDE Systems

In this paper we consider a problem of parameter estimation for a class of partial differential equations that describe the thermal fluid systems in heat exchangers. We employ a "full-flux" physics model, which means the model is defined by coupled convection-diffusion equations where the diffusion coefficient $\mu \geq 0$ is assumed to be "small" when compared to the convection coefficient $v \geq 0$. By setting $\mu = 0$, the hyperbolic equations are viewed as one particular form of the model. We consider the case where one assumes this parameterized model is a source of model discrepancy and measurement errors are a source of noise. In addition, physical considerations can be used to define bounds on the parameters so that the parameter estimation problem becomes a constrained optimization problem. We use a basic counter flow heat exchanger to compare the results obtained from constrained and unconstrained opti-

mization.

John A. Burns, Eugene Cliff
Virginia Tech
Interdisciplinary Center for Applied Mathematics
jaburns@vt.edu, ecliff@vt.edu

Terry L. Herdman
Interdisciplinary Center for Applied Mathematics
Virginia Tech
terry.herdman@vt.edu

MS21

Stabilization by Sparse Controls for a Class of Semilinear Parabolic Equations

Stabilization problems for parabolic equations with polynomial nonlinearities are investigated in the context of an optimal control formulation with a sparsity enhancing cost functional. This formulation allows that the optimal control completely shuts down once the trajectory is sufficiently close to a stable steady state. Such a property is not present for commonly chosen control mechanisms. To establish these results it is necessary to develop a function space framework for a class of optimal control problems posed on infinite time horizons, which is otherwise not available.

Eduardo Casas
Universidad de Cantabria
ETSI Ind y de Telecomm
eduardo.casas@unican.es

Karl Kunisch
Karl-Franzens University Graz
Institute of Mathematics and Scientific Computing
karl.kunisch@uni-graz.at

MS21

Finite Element Discretizations of an Optimal Control Problem Related to the Allen-Cahn Equation

An optimal control problem for the Allen-Cahn equation is considered. In particular, a tracking type functional is minimized subject to the Allen-Cahn equation. The control is of distributed type, and can satisfy point-wise constraints. The proposed fully-discrete scheme is based on a discontinuous (in time) Galerkin scheme, combined with standard finite element discretizations in space. Stability estimates are discussed, and the (polynomial) dependence of various constants upon the parameter $1/\epsilon$ is tracked. Convergence of fully-discrete approximations is also demonstrated under minimal regularity assumptions on the data without imposing any restriction between the temporal and spacial discretization parameters. Finally, error estimates are presented, under mild conditions between the temporal and spacial discretization parameters and the parameter ϵ.

Konstantinos Chrysafinos
Department of Mathematics
National Technical University of Athens, Greece
chrysafinos@math.ntua.gr

MS21

Optimal Control of PDEs with Controls from a Lower Dimensional Manifold and its Approxima-tions

In this talk we introduce some elliptic optimal control problems with controls acting on a lower dimensional manifold which can be a point, a curve or a surface, depending on the dimension of spatial domain. We derive the first order optimality condition and characterize the precise regularity of solutions for different cases. We also consider the finite element discretization with piecewise linear finite elements to approximate state variables, while utilizing the variational discretization to approximate control variables. We derive several a priori error estimates for optimal controls from different cases depending on the dimensions of the computational domain and the manifold where controls act. The nontrivial extensions to time-dependent case are also discussed. At last we provide several numerical experiments which confirm our theoretical findings.

Wei Gong
Institute of Computational Mathematics
Chinese Academy of S
wgong@lsec.cc.ac.cn

MS22

On the Qualitative Properties of the Singularities of Solutions to Hamilton-Jacobi Equations

This talk is based on the joint work with Piermarco Cannarsa and Albert Fathi. We will talk on the propagation of singularities along the generalized characteristics differential inclusions. In particular, we will discuss the asymptotic behavior of the singularities along the generalized characteristics and its connection to the regular dynamics, and also the topological consequence from this approach.

Wei Cheng
Nanjing University
chengwei@nju.edu.cn

MS22

Control Problems in the Wasserstein Space and Applications to Multi-agent Systems

We introduce and study some optimal control problems in the space of probability measures endowed with the Wasserstein distance, where the dynamics is given by a controlled continuity equation.The main motivation is to face situations in finite-dimensional control systems evolving deterministically where the initial position of the controlled particle is not exactly known, but can be expressed by a probability measure on $\mathbf{R}^d$, or to describe at a macroscopical level the behaviour of multi-agent systems, i.e., systems where the number of agents is so high to make unpractical a description of the behaviour of each single agent, while only a statistical description of some parameters of the systems (e.g. the densities of the agent in the space) is feasible. We define also a suitable value function for such problems, which solves an infinite-dimensional Hamilton-Jacobi-Bellman equation in a suitable viscosity sense.

Antonio Marigonda
University of Verona
antonio.marigonda@univr.it

Giulia Cavagnari
Department of Mathematical Sciences
Rutgers University-Camden

giulia.cavagnari@rutgers.edu

MS22
Compactness Estimate for Hamilton-Jabobi Equations

This talk will be devoted to a fundamental question on the compactness of sets of solutions. The key concept in this study is the Kolmogorov epsilon-entropy which is the logarithm of the minimum number of elements in an epsilon-covering of a given (totally bounded) set. I will use this concept to provide a sharp estimate on minimum number of bits needed to represent a viscosity solution of Hamilton-Jacobi equations with accuracy epsilon.

Tien Khai E. Nguyen
North Carolina State University
khai@math.ncsu.edu

MS22
Global Results for Eikonal Hamilton-Jacobi Equations on Networks

This talk is based on a joint work with Antonio Siconolfi. We study a one-parameter family of Eikonal Hamilton-Jacobi equations on an embedded network, and prove that there exists a unique critical value for which the corresponding equation admits global solutions, in a suitable viscosity sense. Such a solution is identified, via an Hopf-Lax type formula, once an admissible trace is assigned on an intrinsic boundary. The salient point of our method is to associate to the network an abstract graph, encoding all of the information on the complexity of the network, and to relate the differential equation to a discrete functional equation on the graph. Comparison principles and representation formulae are proven in the supercritical case as well.

Alfonso Sorrentino
University of Rome "Tor Vergata"
sorrentino@mat.uniroma2.it

MS23
Applications of Nonconvex Sweeping Processes to Real Life Problems

In this talk, I will present my recent results on the use of nonconvex sweeping process in two different real life problems. First, I will present the application to non avoidance of swarm robots. The second application is the simulation of the motion of nanoparticles in straight tubes.

Messaoud Bounkhel
Department of Mathematics
King Saud University, Saudi Arabia
bounkhel@ksu.edu.sa

MS23
Optimal Treatment Strategies for Control Model of Psoriasis

Psoriasis is an autoimmune disorder with the symptoms of chronic inflammation of the skin. Psoriasis causes skin cells to build up quickly on the skin surface, which makes the skin appear red, dry with scaly patch. Adequate treatment for psoriasis is very challenging, and a total cure of the disease still does not exist. Mathematical models have long been effective means to predict cellular behaviors of the skin regulation for a normal or pathological circumstance. In this talk, a proposed control model of psoriasis skin disease is described on a given time interval by a nonlinear control system of three differential equations involving the concentrations of dendritic cells (tissues macrophages), T-lymphocytes and keratinocytes with medication intake as a control function. An optimal control problem of minimizing the release of keratinocytes at the end of the time interval is stated and studied using the Pontryagin maximum principle. Different types of the optimal control in dependence on models parameters are obtained analytically. Numerical simulations of the optimal solutions at these parameters are presented. Possible applications to an optimal drug therapy are discussed.

Ellina V. Grigorieva
Texas Woman's University
Department of mathematics and computer sciences
egrigorieva@twu.edu

Evgenii Khailov
Moscow State University
khailov@cs.msu.su

MS23
A Bilevel Coordination Control Scheme for the Sustainable Management of Renewable Resources

This presentation concerns a control scheme that ensures short term economic sustainability while preserving the long term environment sustainability in the context of a system with multiple distributed often competing and interacting decision makers. The overall problem is organized in a hierarchic control and decision-making structure which involves:

1 A high level model predictive control scheme approximating infinite horizon approximation that defines the feedback-based coordinating strategies for the various producers.

2 Low level dynamic optimization problems to support the producers decision-making in targeting maximal economic returns while subject to various constraints.

Besides the conditions under which the existence of solution to the overall problem, we address challenges concerning the stability and robustness of the coordinating Model Predictive Control (MPC) scheme approximating the infinite horizon optimal control. The derivation of the necessary conditions of optimality for the infinite horizon open loop dynamic optimization problem underlying the MPC scheme - for which we remark that the cost functional depends only on the equilibrium of the system's state at infinity - is also discussed. One key feature of the maximum principle is a novel type of transversality conditions that avoid the degeneracy effect inherent to the infinite horizon under reasonable assumptions on the problem's data.

Fernando L. Pereira
Porto University
flp@fe.up.pt

MS23
Optimal Control Applied to Delayed HIV Models

Time delays play an important role in the dynamics of HIV infection. We propose and investigate two delayed models that study the relationship between HIV and the immune system during the natural course of infection and in the context of antiviral treatment regimes. Sufficient criteria

for local asymptotic stability of the infected and viral free equilibria are given. For each delayed HIV mathematical model, an optimal control problems with time delays both in state variables and control is formulated and analyzed. We compare the extremal of our optimal control problems with state and control delays with the solutions of the associated uncontrolled problems and the control problems with delay in the state variable only.

Cristiana J. Silva
University of Aveiro
cjoaosilva@ua.pt

MS24
Exploiting Low-dimensional Active Subspaces in Design under Uncertainty

Optimization formulations of design under uncertainty have two distinct sets of variables: random variables representing uncertainty and variables that the control the design. Objective and constraint functions are statistics of random performance metrics, where randomness originates from the random variables. These statistics are high-dimensional integrals in the space of random variables, and optimization occurs over the high-dimensional design space. We show how to exploit low-dimensional active subspaces in the combined random/design variable space to estimate design-under-uncertainty solutions efficiently.

Paul Constantine
Colorado School of Mines
Applied Mathematics and Statistics
pconstan@mines.edu

Jeffrey M. Hokanson
Colorado School of Mines
hokanson@mines.edu

Rick Fenrich, Victorien Menier
Stanford University
rfenrich@stanford.edu, menier@stanford.edu

Juan J. Alonso
Department of Aeronautics and Astronautics
Stanford University
jjalonso@stanford.edu

MS24
The Million Point Computational Optimal Control Challenge

It is possible to frame certain graph-theoretic optimization problems as nonsmooth optimal control problems. A key mathematical construct that allows this problem formulation is the Kronecker indicator function defined over a real-valued label space. Through the use of Urysohn's Lemma and C^∞ approximations to the indicator function, it is possible to generate smooth approximations to the nonsmooth optimal control problem. In order to solve the resulting smooth or nonsmooth optimal control problem numerically, it is necessary to generate a discretization level of sufficiently fine granularity to enable a nonzero sampling of the bump functions. This procedure generates a very large-scale computational optimal control problem that can be of the order of a million points in time steps. In this paper, we will present all the mathematical details leading up to this computational challenge. We will also show that the barriers are far less technological (e.g., computer hardware) and more in the realm of new mathematical al-gorithms. If these algorithms can be developed, it holds the potential to revolutionize numerical techniques for solving dynamic graph problems.

Isaac Ross
Naval Postgraduate School
imross@nps.edu

Mark Karpenko
Department of Mechanical and Astronautical Engineering
Naval Postgraduate School
mkarpenk@nps.edu

Ronald Proulx
Control and Optimization Laboratories
Naval Postgraduate School
rjproulx@nps.edu

MS24
A Chaotic Dynamical System that Paints and Samples

Can a dynamical system paint masterpieces such as Da Vinci's Mona Lisa or Monet's Water Lilies? Moreover, can this dynamical system be chaotic in the sense that although the trajectories are sensitive to initial conditions, the same painting is created every time? Setting aside the creative aspect of painting a picture, in this work, we develop a novel algorithm to reproduce paintings and photographs. Combining ideas from ergodic theory and control theory, we construct a chaotic dynamical system with predetermined statistical properties. If one makes the spatial distribution of colors in the picture the target distribution, akin to a human, the algorithm first captures large scale features and then goes on to refine small scale features. Beyond reproducing paintings, this approach is expected to have a wide variety of applications such as uncertainty quantification, sampling for efficient inference in scalable machine learning for big data, and developing effective strategies for search and rescue. In particular, our preliminary studies demonstrate that this algorithm provides significant acceleration and higher accuracy than competing methods for Markov Chain Monte Carlo (MCMC). Additionally, we present convergence proofs for the sampling approach.

Amit Surana
System Dynamics and Optimization
United Tecnologies Research Center (UTRC)
suranaa@utrc.utc.com

MS24
Taylor Approximation for PDE-constrained Optimal Control Problems under High-dimensional Uncertainty: Application to a Turbulence Model

In this talk, we present an efficient method based on Taylor approximation for PDE-constrained optimal control problems under high-dimensional uncertainty. The computational complexity of the method does not depend on the nominal but only on the intrinsic dimension of the uncertain parameter, thus the curse of dimensionality is broken for intrinsically low-dimensional problems. Further correction for the Taylor approximation is proposed, which leads to an unbiased evaluation of the statistical moments in the objective function. We apply our method for a turbulence model with infinite-dimensional random viscosity.

Umberto Villa
University of Texas at Austin

uvilla@ices.utexas.edu

MS25

Weak Formulation of Mean-field Control and Zero-sum Game Problems

This talk is related to the weak formulation of the mean-field control problem and the mean-field zero-sum differential game as well. We show existence of an optimal control and a saddle-point for respectively the control problem and zero-sum differential game associated with payoff functionals of mean-field type, under dynamics driven by weak solutions of stochastic differential equations of mean-field type.

Said Hamadene
University of Le Mans
said.hamadene@univ-lemans.fr

MS25

Optimal Stopping, Smooth Pasting and the Dual Problem

We will consider the problem of optimally stopping a function of a general Markov process (and suitable path functionals) in continuous time. We will show under very general conditions that if the gain function is in the domain of the martingale generator then so is the optimal payoff. We will give applications to the so-called smooth pasting condition and to the dual problem.

Saul Jacka, Dominic Norgilas
Statistics Dept, University of Warwick
s.d.jacka@warwick.ac.uk, d.norgilas@warwick.ac.uk

MS25

Portfolio Optimization Problems for Models with Delays

In the real world, the historical performance of a stock may have impacts on its dynamics and this suggests us to consider models with delays. In this paper, we consider a portfolio optimization problem of Mertons type in which the risky asset is described by a stochastic delay model. We derive the Hamilton-Jacobi-Bellman (HJB) equation, which turns out to be a nonlinear degenerate partial differential equation of the elliptic type. Despite the challenge caused by the nonlinearity and the degeneration, we establish the existence result and the verification results.

Tao Pang
Department of Mathematics
North Carolina State University
tpang@ncsu.edu

MS25

Open-loop and Closed-loop Optimal Controls for Linear-quadratic Problems with Mean-field

Optimal control problem is considered for a mean-field linear stochastic differential equation with a quadratic functional. Open-loop optimal control and closed-loop optimal strategy are introduced, whose existence are characterized by the solvability of an associated system of forward-backward stochastic differential equations and a system of Riccati equations, respectively.

Jiongmin Yong

University of Central Florida
jiongmin.yong@ucf.edu

MS26

A Weak Convergence Approach to Inventory Control using a Long-term Average Criterion

This paper continues the examination of inventory control in which the inventory is modelled by a diffusion process and a long-term average cost criterion is used to make decisions. The class of such models under consideration have general drift and diffusion coefficients and boundary points that are consistent with the notion that demand should tend to reduce the inventory level. The conditions on the cost functions are greatly relaxed from those in Helmes et al (2017). Characterization of the cost of a general (s, S) policy as a function of two variables naturally leads to a nonlinear optimization problem over the ordering levels s and S. Existence of an optimizing pair (s_*, S_*) is established for these models under very weak conditions; non-existence of an optimizing pair is also discussed. Using average expected occupation and ordering measures and weak convergence arguments, weak conditions are given for the optimality of the (s_*, S_*) ordering policy to be optimal in the general class of admissible policies. This approach provides an analytical solution to the problem rather than a solution involving intricate analysis of the stochastic processes. The range of applicability of these results is illustrated on several examples.

Richard Stockbridge
University of Wisconsin - Milwaukee
stockbri@uwm.edu

Kurt Helmes
Humboldt University of Berlin
helmes@wiwi.hu-berlin.de

Chao Zhu
University of Wisconsin-Milwaukee
zhu@uwm.edu

MS26

Finite Element Methods for Linear Programming Formulations in Stochastic Control

This presentation considers formulations of control problems for stochastic processes, including singular behavior, as infinite-dimensional linear programs over a space of expected occupation measures. Numerical approximations to such linear programs offer an alternative to established numerical techniques for stochastic control. The basic approach involves the discretization of an operator-integral equation in style of the finite element method. Then, the occupation measures are approximated by finite linear combinations of point masses and integrable functions. Finally, classic solvers for linear programs are used to generate an approximate solution to the control problem. A convergences analysis is given to show the validity of this approach. Its performance is illustrated by an exemplary stochastic control problem.

Martin Vieten
University of Wisconsin-Milwaukee
Department of Mathematical Sciences

mgvieten@uwm.edu

MS26
Stochastic Control with Running Max Costs

Motivated by the efficient control of an infinite server processing system under heavy traffic conditions, here we consider a drift rate control problem represented by a stochastic differential equation(SDE) model. The associated cost structure constitute of two types of costs: a convex control cost and a linear cost proportional to the growth of the running maximum. We formulate the associated HJB equation, which is a degenerate equation with a Neumann boundary condition on an unbounded domain. We obtain an optimal strategy for the SDE control problem by constructing a solution to the HJB equation. Using this solution, an asymptotically optimal strategy is derived for the infinite-server controlled processing system.

Ananda Weerasinghe
Iowa State University
Department of Mathematics
ananda@iastate.edu

MS26
Exact Controllability of Linear Stochastic Differential Equations and Related Problems

A notion of L^p-exact controllability is introduced for linear controlled (forward) stochastic differential equations (FSDE, for short). Inspired by the deterministic cases, it is shown that the L^p-exact controllability of an FSDE is equivalent to the validity of an L^q-observability inequality for the adjoint equation of the original state equation, which is a linear backward stochastic differential equation (BSDE, for short), with $\frac{1}{p} + \frac{1}{q} = 1$. Further, a stochastic norm optimal control problem is investigated, whose solvability is equivalent to the L^p-exact controllability of the corresponding FSDE control system. In addition, for FSDE with deterministic coefficients, some useful sufficient conditions of L^p-exact controllability are established.

Jiongmin Yong
University of Central Florida
jyong@mail.ucf.edu

MS27
Optimizing Stimulation to Suppress Pathological Neural Oscillations

Control theory approaches can be used to optimize electrical stimulus design to modulate physiological activity associated with disease. High frequency deep brain stimulation is used to treat motor symptoms of Parkinsons disease (PD). While effective, improved stimulation designed to specifically target physiological signals underlying symptoms may improve efficacy and reduce side effects. Enhanced oscillatory activity in the beta frequency range (12-30 Hz) is thought to underlie motor symptoms in PD. Here we propose to use a simple model characterizing the interaction between a stimulus pulse and the neural oscillation to optimize the timing of stimuli to disrupt pathological oscillatory activity. Stimulation causes shifts in the phase of enhanced beta oscillations seen in animal models of PD and PD patients. Phase response curves (PRCs) can be used to characterize these shifts and make predictions about how the oscillatory signal will respond to stimulation parameters, such as stimulus phase. While PRCs are

well described for single neurons, chronic recordings from patients require the use of field potential recordings. Here I describe methods for estimating the PRC from field potential recordings and show how population PRCs can be used to identify stimulus parameters to suppress oscillatory activity. While the focus here is on oscillatory activity in Parkinsons disease, this approach can be used to enhance or suppress any oscillatory neurological signal.

Abbey Holt, Andrew Sharott
University of Oxford
abbey.becker@pharm.ox.ac.uk, andrew.sharott@pharm.ox.ac.uk

MS27
Clustered Desynchronization of Neural Oscillators

Inspired by the hypothesis that some symptoms of Parkinson's disease are related to pathological synchronization in the motor control region of the brain, there has been interest in finding electrical stimuli which desynchronize neural populations. Recent results on coordinated reset and periodically forced oscillators suggest that forming distinct clusters of neurons may prove to be more effective than achieving complete desynchronization, in particular by promoting plasticity effects that might persist after stimulation is turned off. We propose a single-input low-power control strategy to achieve such clustering, based on the analysis of the reduced phase model for a set of identical neurons.

Jeff Moehlis, Timothy Matchen
Dept. of Mechanical Engineering
University of California – Santa Barbara
moehlis@engineering.ucsb.edu, tmatchen@umail.ucsb.edu

MS27
Defining Suitable Control Objectives for Sensory Prostheses

Most theories of neural coding in sensory systems suppose neuron identity carries information, but overall function arises from large ensembles (e.g. $\sim 10^4$ neurons in a cortical column). From a control perspective, it can be difficult to define objectives for a neurostimulating sensory prosthesis at this intermediate scale, where bulk changes are not sufficient (in contrast to, e.g., desynchronizing deep brain stimulation), but the number of "individual' neurons requiring manipulation is too large to lead to controllability in a traditional sense. Of particular importance is that currently realizable technology is highly underactuated: the dynamical dimension of the neural network is much larger than the number of independent channels of stimulation. I will describe our efforts towards bridging control theory with *in vivo* neurophysiology. We exploit neural heterogeneity to design controls for ensembles that are naively uncontrollable. We argue that achieving robustness may motivate intentional model misspecification, and reconsideration of the definitions of controllability for a neural ensemble. For example, biophysical objectives might be relaxed in favor of coding variables in a sensory application. The latter point is highlighted by our initial efforts to merge the analysis with *in vivo* recording and stimulation in mouse somatosensory cortex.

Jason Ritt
Boston University
jritt@bu.edu

ShiNung Ching
Washington University in St. Louis
shinung@ese.wustl.edu

MS27

Optimal Entrainment of Neurons in Uncertain and Noisy Environments

Classical optimal control techniques which rely on the minimization of a cost functional usually require nearly perfect knowledge of an underlying deterministic system. However, despite our best efforts, noise, uncertainty, and heterogeneity are unavoidable features of living neurological systems; these features have the tendency to undermine the efficacy of resulting optimal control policies. This work focuses on a methodology to design an optimal strategy to entrain a population of nonlinear, noisy limit cycle oscillators with uncertain properties. Illustrations in numerical models of noisy phase oscillators and *in vitro* hippocampal neurons are given. Because this control strategy explicitly accounts for the noise and uncertainty that are unavoidable in living systems, it could have relevance in neural pathways where robust spike timing is important.

Dan D. Wilson
Mathematics
University of Pittsburgh
dan.d.wilson8@gmail.com

Jeff Moehlis
Dept. of Mechanical Engineering
University of California – Santa Barbara
moehlis@engineering.ucsb.edu

MS28

Koopman-based Control-oriented Bilinear System Identification

Integrating system inputs into the Koopman operator framework would enable the development of linear but globally valid controllers and estimators for a range of nonlinear systems of interest in practical applications. Recent advances in Koopman operator theory have led to the formulation of a bilinear Koopman Observer Form (KOF), which represents the underlying nonlinear system with a bilinear system that can be used for estimator or control design. This presentation focuses on the computation of bilinear KOF from data using standard Koopman Modal Decomposition (KMD) for autonomous systems in combination with a known method from bilinear system identification, Single Experiment with Multiple Pulses (SEMP). We first demonstrate the accuracy of the combined identification method on an analytical example where the bilinear KOF can be computed exactly and proceed to apply it to a controlled version of the van der Pol oscillator.

Milos Ilak
UTRC
ilakm@utrc.utc.com

Matthew Williams
United Technologies Research Center
william1@utrc.utc.com

Amit Surana
System Dynamics and Optimization
United Tecnologies Research Center (UTRC)

suranaa@utrc.utc.com

MS28

Linear Predictors for Nonlinear Dynamical Systems: Koopman Operator Meets Model Predictive Control

This talk presents an extension of theKoopman operator theory to controlled dynamical systems with the aim at feedback controller design for nonlinear dynamical systems. Applying a modifiedversion of the extended dynamic mode decomposition to compute a finite-dimensional approximation to the Koopman operator leads to a predictor of the form of a controlled linear dynamical system.In numerical examples, predictors obtained in this wayexhibit a performance superior to existing linear predictors such as those based on local linearization orCarleman linearization. These linear predictors can be readily used to design controllers for the nonlinear dynamical system using linear controller design methodologies. We focus in particular on model predictive control (MPC) and show that an MPC controller designed in this way enjoys a computational complexitycomparable to that of MPC for a linear dynamical system with the same number of control inputs and the same dimension of the state-space.

Milan Korda
University of California at Santa Barbara
USA
korda.m@gmail.com

Igor Mezic
UCSB
mezic@engr.ucsb.edu

MS28

Adapting Koopman Operator Theory to Handle Modern Infectious Disease Data

Data-driven, equation-free techniques are rapidly gaining popularity in the analysis and modeling of complex systems. Equation-free techniques predominantly rely on measurement data, bypassing the need for governing equations based on first principles. With the rapidly increasing collection of data from biological systems such as infectious disease spread, equation-free techniques, such as Koopman operator theory, are poised to both characterize the underlying nonlinear dynamics and design control strategies. Modern data from infectious disease spread poses a challenge, though, to Koopman modal decomposition: measureable disease interventions such as vaccination or bednet campaigns are exogenous forcing. Standard Koopman analysis and DMD are incapable of producing input-output models; moreover, external forcing will corrupt the dynamics and the modes. In this talk, I will discuss a new generalization of Koopman operator theory that incorporates the effects of inputs and control. Further, I will show how this generalization is rigorously connected and generalizes a recent development called Dynamic Mode Decomposition with control.

Joshua L. Proctor
Institute for Disease Modeling
JoshLProctor@gmail.com

MS29

Plasmo: A Platform for Scalable Modeling and Op-

timization

PLASMO (Platform for Scalable Modeling and Optimization) is a Julia-based open-source software platform that facilities the construction, solution, instantiation, and management of large-scale optimization problems on high-performance computers. We discuss how to use the platform to target problems in stochastic programming formulations, integrated planning/scheduling/control, and multi-scale/hierarchical networks. For instance, PLASMO can be used to express hierarchical networks as trees where each node represents a component or a network itself. Each node has its own model, objective function, and connectivity of its children. In this way, PLASMO allows highly compact and scalable object-oriented expressions of the problem. PLASMO is already interfaced with serial solvers like IPOPT and parallel solvers like PIPS-NLP and DSP. When PIPS-NLP is used, PLASMO enables not only parallel model instantiation but also parallel evaluation of the Hessian, Jacobian, and objective/constraint functions. Furthermore, we use PLASMO to model a CHP design study and a wind turbine stochastic optimal control problem.

Yankai Cao
University of Wisconsin-Madison
cao27@wisc.edu

Jordan Jalving
University of Wisconsin
jalving@wisc.edu

Kibaek Kim
Mathematics and Computer Science Division
Argonne National Laboratory
kimk@anl.gov

Victor Zavala
University of Wisconsin-Madison
victor.zavala@wisc.edu

MS29

Fast Feedback Multi-stage NMPC Using Structure-Exploiting Numerical Methods

For nonlinear model predictive control (NMPC) Dadhe and Engell [2008] propose the multi-stage approach based on a scenario tree formulation to robustify against possible uncertainties. For large trees representing the uncertainty space the solution of the optimization problems during the NMPC scheme becomes challenging. We have to give fast feedback to ensure real-time applicability of the optimization-based control scheme. By the direct multiple shooting method we discretize the optimal control problems of a NMPC iteration to obtain a sequence of finite-dimensional nonlinear optimization problems. We solve those problems approximately using multi level iterations that can be understood as the iterative application of nonlinear feedback laws implicitly given by the solution of quadratic programming problems (QPs). The occurring QPs exhibit a particular structure originating from the multi-stage formulation. We present a dual decomposition approach on the QP level to exploit the scenario tree structure. As a result we can solve a magnitude of smaller QPs fast and in parallel to obtain the solution of the large tree-structured QP. Finally, we showcase numerical results for a biochemical batch reactor and large scenario trees.

Conrad Leidereiter
IWR, University of Heidelberg
conrad.leidereiter@iwr.uni-heidelberg.de

Andreas Potschka
Interdisciplinary Center for Scientific Computing
University of Heidelberg
potschka@iwr.uni-heidelberg.de

Hans Georg Bock
IWR, University of Heidelberg
bock@iwr.uni-heidelberg.de

MS29

PYOMO.DAE: A Python-based Framework for Dynamic Optimization

Dynamic optimization problems include differential equations as constraints and allow users to incorporate dynamic models directly within an optimization framework. However, implementing and solving this class of optimization problem is challenging, particularly for non-experts, due to the reformulations that must be applied in order to solve these problems using general algebraic optimization solvers. Pyomo.dae is a modeling package meant to address this challenge by allowing users to formulate dynamic optimization problems using a natural and intuitive syntax and providing general implementations of reformulations which can be used to automatically generate algebraic approximations of dynamic models that can be solved using off-the-shelf optimization solvers. This talk gives an overview of the dynamic optimization modeling flexibility provided by pyomo.dae and the included reformulations. In addition, we discuss new features being developed for the package and demonstrate pyomo.dae on a variety of examples. Finally, we show how pyomo.dae can be combined with other Pyomo modeling extensions, such as PySP for stochastic programming, in order to quickly and concisely implement and solve sophisticated, cutting-edge optimization problems incorporating dynamics.

Bethany Nicholson
Sandia National Laboratories
blnicho@sandia.gov

John D. Siirola
Sandia National Laboratories
Exploratory Simulation Technologies
jdsiiro@sandia.gov

MS29

Parallel Cyclic Reduction Decomposition for Dynamic Optimization Problems

Direct transcription of dynamic optimization problems, with differential-algebraic equations discretized and written as algebraic constraints, creates very large nonlinear optimization problems. When this discretized optimization problem is solved with an NLP solver, such as IPOPT, the dominant computational cost often lies in solving the linear system that generates Newton steps for the KKT system. Computational cost and memory constraints for this linear system solution raise many challenges as the system size increases. On the other hand, the linear KKT system is sparse and structured, and can be permuted to form a block tridiagonal matrix. This talk explores a parallel decomposition strategy for block tridiagonal systems that is based on cyclic reduction (CR) factorization of the KKT matrix. The classical CR method is based on repeated Schur complement factorizations, has good observed per-

formance, but its numerical stability properties are unproved for our KKT system. Alternately, Yalamov and Pavlov proposed a modified, full-space CR algorithm with proven stability bounds. Here we compare the performance of both methods on random test matrices. Stable behavior is observed in both cases, and the classical CR method has lower computational cost. This result is justified by analyzing the complexity of both methods. Finally, we discuss modifications to the CR decomposition that improve performance, and we apply the approach to an industrially relevant problem.

Wei Wan
Chemical Engineering Department
Carnegie Mellon
weiwan@andrew.cmu.edu

Bethany Nicholson
Sandia National Laboratories
blnicho@sandia.gov

Lorenz Biegler
Carnegie Mellon University
Department of Chemical Engineering
lb01@andrew.cmu.edu

MS30

Optimality Conditions in an Infinite Horizon Optimal Control Problem in Discrete Time

This talk is devoted to the study of an infinite horizon optimal control problem with discounting in discrete time. We introduce an infinite-dimensional linear programming problem (IDLP) closely related to this problem. We derive necessary and sufficient conditions of optimality for the optimal control problem in terms of the solution of the dual to the IDLP. We also obtain asymptotic relations between the value functions in the problems with discounting and long-run average criteria. The talk is based on the joint work with V.Gaitsgory and A. Parkinson.

Ilya Shvartsman
Penn State Harrisburg
Middletown, PA
ius13@psu.edu

MS30

Regularization of Pontryagin Maximum Principle in Optimal Control with Pointwise State Constraints

We consider the "simplest" convex optimal control problem with pointwise equality and inequality state constraints for the system of ordinary differential equations and discuss how to overcome the instability of the classical optimality conditions in the way of applying dual regularization method and simultaneous transition to the concept of minimizing sequence of admissible elements as the main concept of optimization theory. The main attention in the talk is given to the discussion of the so-called regularized or, in other words, stable, with respect to perturbation of input data, sequential Lagrange principle in the nondifferential form and Pontryagin maximum principle. Regardless of the stability or instability of the original optimal control problem, they stably generate minimizing approximate solutions in the sense of J. Warga for it and thus, they are regularizing algorithms in this problem. For this reason, we can interpret them as tools for direct solving unstable optimal control problems.

Mikhail Sumin
Department of Mathematics
University of Nizhnij Novgorod
m.sumin@mail.ru

MS31

Computation and Evaluation of Nonlinear Feedback in a Flow Control Problem

When computable, a linear feedback control guarantees the stability of a steady-state flow. However in many cases the stability region might be too small to be implemented in practice. This motivates the use of nonlinear feedback strategies to expand the stability region. These can now be efficiently computed using the nonlinear systems toolbox on very low-dimensional, reduced-order models. We explore the expansion of the stability regions for a feedback flow control problem when using either linear or nonlinear feedback gains from the linearized or quadratic system, respectively. We build the feedback law for the linearized system using interpolatory model reduction techniques while using the popular proper orthogonal decomposition method to produce a low-order quadratic model that is small enough to apply the nonlinear systems toolbox created by Art Krener. The effectiveness of the two control laws are tested on a challenging feedback flow control problem involving flow past an array of cylinders.

Jeff Borggaard
Virginia Tech
Department of Mathematics
jborggaard@vt.edu

MS31

Identification of Dynamical Systems with Structured Uncertainty

In this paper we consider the problem of parameter identification for models defined by infinite dimensional dynamical systems with structured uncertainty. This type of problem often occurs in engineering and we show how parameter estimation can be improved by taking advantage of the specific structure of the model form. We discuss approaches to deal with model discrepancy when the systems are described by classes of parameterized PDE models. The results are applicable to problems where, in the process of modeling a complex system, one ignores "small' parameters to obtain simplified models and when infinite dimensional systems are approximated. We show for these common sources of model discrepancies, hierarchical modeling can be employed to aid in the development of prior knowledge about the model form caused by uncertain or ignored parameters. We focus on a special class of inverse problems for PDE control systems and present two methods to help deal with model discrepancy. An application to modeling and control of a thermal fluid system is presented to illustrate the ideas.

John A. Burns, Eugene Cliff
Virginia Tech
Interdisciplinary Center for Applied Mathematics
jaburns@vt.edu, ecliff@vt.edu

MS31

Using Modified Centroidal Voronoi Tessellations for Sensor Selection and State Feedback Kernel

Partitioning in Parabolic PDEs

This work continues on earlier work on the use of CVT for sensor location selection in the compensator design of parabolic PDEs. Instead of using the feedback kernel as the density function to obtain the mass centroid, the proposed approach ensures that the sensor location in a given cell is such that it subsequently divides the cell into two subcells of equal areas of the feedback kernel. The resulting optimal sensor location is used in conjuction with an output feedback controller as a means to implement a computational scheme to reduce an optimal full-state feedback controller into a suboptimal static output feedback controller.

Michael A. Demetriou
Worcester Polytechnic Institute
mdemetri@wpi.edu

MS31
Boundary Control of Optimal Mixing in Stokes Flows

We discuss the optimal boundary control problem for mixing an inhomogeneous distribution of a passive scalar field in an unsteady Stokes flow. The problem is motivated by mixing the fluids within a cavity or vessel at low Reynolds numbers by moving the walls or stirring at the boundaries. It is natural to consider the velocity field which is induced by a control input tangentially acting on the boundary of the domain through the Navier slip boundary conditions. Our main objective is to design an optimal Navier slip boundary control that optimizes mixing at a given final time. This essentially leads to a finite time optimal control problem of a bilinear system. A rigorous proof of the existence of an optimal controller and the first-order necessary conditions for optimality are presented.

Weiwei Hu
University of Southern California
weiwei.hu@okstate.edu

Weiwei Hu
Oklahoma State University
weiwei.hu@okstate.edu

MS32
Optimal Boundary Control Problems with Hyperbolic Systems: The Turnpike Phenomenon

We study the turnpike phenomenon for optimal boundary control problems with hyperbolic systems. We show that for with increasing time horizon the solution of a certain static optimal control problem (where time does not appear) comes closer and closer to the solution of the dynamic optimal control problem. We show that also for optimal boundary control problems with switching, the turnpike phenomenon can occur.

Martin Gugat
Friedrich-Alexander-University Erlangen-Nuremberg (FAU)
Germany
martin.gugat@fau.de

MS32
On a Dynamic Boundary Control Game with a Star of Vibrating Strings

Consider a star-shaped network of vibrating strings. Each string is governed by the wave equation. At the central node, the states are coupled by algebraic node conditions in such a way that the energy is conserved. At each boundary node of the network there is a player that performs Dirichlet boundary control action and in this way influences the system state. We consider the corresponding antagonistic game, where each player minimizes her quadratic objective function that is the sum of a control cost and a tracking term for the final state. We show that under suitable assumptions a unique Nash equilibrium exists and give an explicit representation of the equilibrium strategies.

Sonja Steffensen
RWTH Aachen
steffensen@igpm.rwth-aachen.de

Martin Gugat
Friedrich-Alexander-University Erlangen-Nuremberg (FAU)
Germany
martin.gugat@fau.de

MS32
Exponential Stability of Hyperbolic Balance Laws with Characteristic Boundaries

This talk is concerned with boundary stabilization of one-dimensional linear hyperbolic systems with characteristic boundaries. We assume that the systems satisfy a structural stability condition for hyperbolic relaxation problems, which describe various non-equilibrium phenomena. By introducing proper Lyapunov functions, the structural stability condition is used to derive stabilization results for problems with characteristic boundaries. The result is illustrated with an application to the transport of neurofilaments in axons—a phenomenon studied in neuroscience.

Wen-An Yong
Zhou Pei-Yuan Center for Applied Mathematics
Tsinghua University
wayong@mail.tsinghua.edu.cn

MS32
Data-fitted Second-order Macroscopic Production Models for One Junction

We consider a production line with one junction, i.e., it consists of three machines where one machine takes the products from the other two as the input. The discrete event simulations based on the M/M/1-queuing theory are used to analyze the parameters and derive the correlations between three machines. Then we introduce the second-order macroscopic production model with a new variable. We are able to perform the data-fitted modeling to determine the right parameters that ensures the desired behavior of the production line. Proper boundary conditions will be discussed along with the numerical simulations.

Hui Yu, Michael Herty
RWTH Aachen University
hyu@igpm.rwth-aachen.de, herty@igpm.rwth-aachen.de

MS33
Averaging of Control Systems with Slow Observables

We will discuss results about averaging of control systems characterized by that the influence of controls on the dy-

namics of certain functions of state variables (called observables) is relatively weak and the rates of change of these observables are much slower than the rates of change of the state variables themselves. Theoretical results will be demonstrated with a numerical example.

Vladimir Gaitsgory
Department of Mathematics
Macquarie University Sydney
vladimir.gaitsgory@mq.edu.au

MS33

Optimal Control Problems with Discontinuous Right Hand Side

In this talk we consider optimal control problems with differential equations systems where right hand side may have discontinuities not only in states but also in controls. Optimal control of systems of differential equations with discontinuous right hand side are widely used to describe numerous applications in natural sciences and engineering, where e.g. there is a necessity to model dynamics with different scales or or with jumps. Moreover, optimal control problems with integer controls may be viewed as a special case of the considered optimal control problems. We show that application of Filipov rule for such optimal control problems may still lead to incorrect problems and discuss how to reformulate the problems in proper way. Using the reformulated problem we may prove new necessary optimality conditions. Furthermore we analyze how based on the solution of the reformulated problem to construct the approximation to the solution of original problem for any given accuracy. This is a joint work with Olga Kostyukova.

Ekaterina Kostina
Heidelberg University
ekaterina.kostina@iwr.uni-heidelberg.de

MS33

One-dimensional Non-autonomous Integral Functionals with Discontinuous Non-convex Integrands: Lipschitz Regularity and DuBois-Reymond Necessary Conditions

A famous result by Clarke and Vinter (1985) asserts the Lipschitz regularity of the minimizers of an autonomous one-dimensional Lagrange problem of the calculus of variations. The result was refined by Dal Maso and Frankowska (2003) for Lagrangeans that are just Borel. In both cases the Nagumo superlinear growth condition yields lipschitzeanity of the minimisers. In a joint paper with P. Bettiol we extend the result to a class of non-autonomous Lagrangeans. Under a local Lipschitz condition on the independent variable t we show that the minimizers of

$$\min \int_a^b L(t, x(t), x'(t))\, dt,\ x \in AC[a,b],\ x(a) = A, x(b) = B$$

satisfy a new Weierstrass-like necessary condition. Lipschitzeanity of the minimizers is then obtained under a weaker growth condition than Nagumo. Our methods involve Clarke's more recent formulations of the maximum principle.

Carlo Mariconda
Università degli Studi di Padova
carlo.mariconda@unipd.it

MS33

Optimality Conditions for a Controlled Sweeping Process with Applications to the Crowd Motion Model

The talk concerns the study and applications of a new class of optimal control problems governed by a perturbed sweeping process of the hysteresis type with control functions acting in both play-and-stop operator and additive perturbations. Such control problems can be reduced to optimization of discontinuous and unbounded differential inclusions with pointwise state constraints, which are immensely challenging in control theory and prevent employing conventional variation techniques to derive necessary optimality conditions. We develop the method of discrete approximations married to appropriate generalized differential tools of modern variational analysis to overcome principal difficulties in passing to the limit from optimality conditions for finite-difference systems. This approach leads us to nondegenerate necessary conditions for local minimizers of the controlled sweeping process expressed entirely via the problem data. Besides illustrative examples, we apply the obtained results to an optimal control problem associated with of the crowd motion model of traffic flow in a corridor, which is formulated in this paper. The derived optimality conditions allow us to develop an effective procedure to solve this problem in a general setting and completely calculate optimal solutions in particular situations. Based on joint research with Tan Cao.

Boris Mordukhovich
Wayne State University
Department of Mathematics
boris@math.wayne.edu

MS34

Motion Tracking Sensors in Watersports as Sampling Platforms in Model-based Data Assimilation Systems for Sea Surface Dynamics

This research uses motion data from ocean sports with on-board tracking devices to estimate the sea surface dynamics (waves and currents) of a specific area. Water athletes depend strongly on model-based forecasts to pursue their activities safely, helping them to choose the appropriate equipment and location. On the other hand, these individuals use more and more sensors while pursuing their activity, but only for personal feedback. In this first study, we want to feed this collected data back into ocean dynamics models to generate better localized models for specific areas of interest. Inertial measurement units and satellite positioning, as used for low-cost autonomous vehicles, are used on-board for motion estimation of sailboats, surfers and kitesurfers. Specific motion models for the different disciplines serve as inverse transfer functions from measurements to sea state, using ensemble Kalman filtering to assimilate the data. Combined with wind measurements, moored sensor buoys, bathymetry of the area, tidal state and forecasts, the goal is to generate an infrastructure to feed back data that is collected casually into localized models for improved forecasts and with the prospect to give real-time feedback to athletes of changing conditions and for sensor-assisted sport coaching.

Axel Hackbarth, Edwin Kreuzer, Eugen Solowjow
Institute of Mechanics and Ocean Engineering
Hamburg University of Technology

axel.hackbarth@tuhh.de,   kreuzer@tuhh.de,   eu-
gen.solowjow@tuhh.de

MS34

The Error of Representation in the Ensemble Kalman Filter

We develop techniques needed to account for representation error in data assimilation. Representation error is a characterization of the mismatch between numerical models and the physical processes they are approximating. We study the relationship of low resolution forecasts with unresolved processes to high resolution forecasts with fully resolved processes. Specifically, we discuss numerical methods for determining a map between the high and low resolution models. We then use the Korteweg-DeVries nonlinear wave model to demonstrate these methods in data assimilation.

Sarah King, Daniel Hodyss
Naval Research Laboratory
sarah.king@nrlmry.navy.mil,
daniel.hodyss@nrlmry.navy.mil

MS34

A Hybrid Filter for Assimilating Lagrangian Data into a High-dimensional Model

We will discuss a hybrid particle-ensemble Kalman filter for assimilating Lagrangian data, and apply it to a high-dimensional quasi-geostrophic ocean model. Effectively this hybrid filter applies a particle filter to the highly nonlinear, low-dimensional Lagrangian instrument variables while applying an ensemble Kalman type update to the high-dimensional Eulerian flow field. We will focus on challenges in applying this filter to a high dimensional problem and compare the hybrid filter and Ensemble Kalman filter on some test cases.

Elaine Spiller
Marquette University
elaine.spiller@marquette.edu

Amit Apte
TIFR Centre for Applicable Mathematics
Bangalore, India
apte@icts.res.in

Laura Slivinski
CIRES, NOAA
laura.slivinski@noaa.gov

MS34

Recent Progress in Motion Tomography: Using Timing Information in Flow Field Construction from Trajectory Data

Motion tomography algorithms combines models of ocean flow filed and measurements of underwater vehicle trajectories to construct a high resolution flow map, which can be used for the real-time guidance of the vehicles. This talk introduces a new motion tomography algorithm that leverages the difference between predicted time of arrival and the measured time of arrival to improve the accuracy of the map. Tomography algorithms are known for multiple solutions. By incorporating time differences, some of the unwanted solutions can be removed so that the algorithm converges to better solutions.

Fumin Zhang
School of Electrical and Computer Engineering
Georgia Institute of Technology
fumin@gatech.edu

Meriam Ouerghi
Georgia Institute of Technology
mouerghi3@gatech.edu

MS35

Investment and Consumption in Regime-switching Models with Proportional Transaction Costs and Log Utility

We present an infinite-horizon problem of optimal investment and consumption with proportional transaction costs in continuous-time regime-switching models. A log utility is considered. Using a combination of viscosity solution to the Hamilton-Jacobi-Bellman (HJB) equation and convex analysis of the value function, we are able to derive the characterizations of the buy, sell and no-transaction regions that are regime-dependent.

Jiapeng Liu
School of Economics and Management
China Jiliang University
jpliu@cjlu.edu.cn

Ruihua Liu
University of Dayton
Department of Mathematics
rliu01@udayton.edu

Dan Ren
University of Dayton
dren01@udayton.edu

MS35

A Complex-valued Controlled-diffusion Representation for the Schrödinger Equation in a Rotating Frame

Using the dequantized form of the Schrödinger equation initial value problem, which takes the form of a Hamilton-Jacobi PDE problem, one may obtain a representation for the solution as the value function of a certain controlled-diffusion process. This value is defined in terms of stationarity rather than optimization. The underlying diffusion process is driven by a real-valued Brownian motion, but takes values in a Euclidean space over the complex field. The payoff is also complex-valued. In the case of a single particle in a symmetric field, it is interesting to transform to a rotating frame. There, one can employ these representations to obtain approximations converging to the solution.

William M. McEneaney
Dept. of Mechanical and Aerospace Engineering
University of California, San Diego
wmceneaney@ucsd.edu

Ruobing Zhao
Univ. of California San Diego

ruz015@eng.ucsd.edu

MS35

Equilibrium Strategies for Time-inconsistent Stochastic Switching Systems

An optimal control problem is considered for a controlled stochastic switching system with a recursive cost functional having some non-exponential discounting. Due to the discounting is non-exponential, the problem is time-inconsistent in general. Instead of finding a global optimal control (which is not possible), we look for a time-consistent locally optimal equilibrium strategy. Such a strategy can be represented by a system of equilibrium Hamilton-Jacob-Bellman (HJB, for short) equations, constructed through a sequence of multi-person differential games. A verification theorem is proved and the well-posedness of the equilibrium HJB equation is established as well.

Hongwei Mei, Jiongmin Yong
University of Central Florida
hongwei.mei@ucf.edu, jiongmin.yong@ucf.edu

MS35

Decentralized Dynamic and H^∞ Control in Power System Frequency Regulation

Traditional power systems commonly use droop control methods to coordinate real power generations to regulate grid frequency. While the droop control does not require communication systems, its performance in attenuating load disturbance is highly limited. By employing only distributed information exchange, this paper introduces new distributed control strategies that employ consensus-type methods to coordinate distributed power generations and H^∞ optimal disturbance attenuation to provide robustness against distributed load disturbances. Theoretical analysis is conducted to derive error bounds on frequency deviations. Case studies are provided to demonstrate performance, benefits,and implementation issues of our methods.

Le Yi Wang, Feixiong Chen
Wayne State University
lywang@ece.eng.wayne.edu, feixiong.chen@wayne.edu

Minyou Chen
Chongqing University
minyouchen@cqu.edu.cn

MS36

Dynamic Pricing with Multiple Order Sizes

Dynamic pricing models often assume that customers order one item at a time. This assumption is generalized to account for customers ordering multiple items at a time. In particular, this generalization is applied to the dynamic pricing model with constant demand elasticity as studied by R.P. McAfee and V. te Velde (POMS, 2008), and comparison results are discussed.

Nyles Breecher
University of Wisconsin-Milwaukee
Department of Mathematical Sciences

breecher@uwm.edu

MS36

Dynamic Pricing with Constant Demand Elasticity: A Diffusion Approximation of the Optimal Inventory Process

The dynamic pricing model with constant demand elasticity, first studied by R.P. McAfee and V. te Velde (POMS, 2008), is further analyzed. A diffusion approximation of the optimal inventory process is developed. The approximation follows from functional central limit theorems for this particular dynamic pricing model. The talk is based on joint work with T. Kurtz and T. Templin.

Kurt Helmes
Humboldt University of Berlin
helmes@wiwi.hu-berlin.de

MS36

On the Limit of Weakly Interacting Stochastic Processes with Markovian Switching

This talk considers asymptotic properties of systems of weakly interacting particles with a common Markovian switching. It is shown that when the number of particles tends to infinity, certain measure-valued stochastic processes describing the time evolution of the systems converge to a stochastic nonlinear process which can be described as a solution to a stochastic McKean-Vlasov equation.

Son L. Nguyen
University of Puerto Rico - Rio Piedras
nluuson@yahoo.com

Tuan Hoang, George Yin
Wayne State University
tuan.hoang@wayne.edu, gyin@math.wayne.edu.

MS36

Asymptotic Properties of Recurrence and Ergodicity of Switching Diffusions with Past-dependent Switching Having a Countable State Space

This work focuses on recurrence, ergodicity, and stability of switching diffusion consisting of continuous and discrete components, in which the discrete component takes values in a countably infinite set and the rates of switching at current time depend on the value of the continuous component over an interval including certain past history. Sufficient conditions for recurrence, ergodicity and stability of the solution process are given. Another distinctive feature of this work is that the path-wise rate of convergence is estimated when the solution is asymptotically stable. Some examples are given to illustrate the findings.

Hai Dang Nguyen
Wayne State University
dang.nguyen@wayne.edu

George Yin
Wayne State University
Department of Mathematics
gyin@math.wayne.edu

MS37

Optimal Control for a Sir Epidemiological Model

with Time-varying Populations

In this talk, an SIR epidemiological model with time varying population is formulated as an optimal control problem. Vaccination and treatment are considered as control variables to manage the outbreak of a disease. We used Pontryagins maximum principle to characterize the optimal levels of the two controls. The theory establishes that optimal vaccination schedule will be concatenations of bang and singular controls while optimal treatment schedules will be bang-bang.

Mahya Aghaee
Department of Mathematics
University of Florida
mahyaaghaee@ufl.edu

Urszula Ledzewicz
Southern Illinois University, USA
uledzew@siue.edu

Heinz M. Schaettler
Dept. of Systems Science and Mathematics
Washington University
hms@cec.wustl.edu

MS37
Cancer Treatment

An optimal control problem for combination of cancer chemotherapy with immunotherapy in form of a boost to the immune system is considered as a multi-input optimal control problem. The objective to be minimized is chosen as a weighted average of (i) the number of cancer cells at the terminal time, (ii) a measure for the immunocompetent cell densities at the terminal point (included as a negative term), the overall amounts of (iii) cytotoxic agents and (iv) immune boost given as a measure for the side effects of treatment and (v) a small penalty on the free terminal time that limits the overall therapy horizon. This last term is essential in obtaining a mathematically well-posed problem formulation. Both analytical and numerical results about the structures of optimal controls will be presented that give some insights into the structure of optimal protocols, i.e., the dose rates and sequencing of drugs in these combination treatments.

Mojdeh Faraji
Bioengineering
Georgia Institute of Technology
mojdeh@gatech.edu

Urszula Ledzewicz
Southern Illinois University, USA
uledzew@siue.edu

Heinz M. Schaettler
Dept. of Systems Science and Mathematics
Washington University
hms@cec.wustl.edu

MS37
Optimal Control of Sugarscape Agent-based Model via a PDE Approximation Model

There is no standard framework for solving optimization problems for systems described by agent-based models (ABMs). We present a method for constructing individual-level controls that steer the population-level dynamics of an ABM towards a desired state. Our method uses a system of partial differential equations (PDEs) with control functions to approximate the dynamics of the ABM with control. An optimal control problem is formulated in terms of the PDE model to mimic the optimization goal of the ABM. Mathematical theory is used to derive optimal controls for the PDE model, which are numerically approximated and transformed for use in the ABM. We use the Sugarscape ABM, a prototype ABM that includes several important biological features. We present a PDE model that approximates well the spatial and temporal dynamics of the Sugarscape ABM. In both models, control represents taxation of agent wealth with the goal to maximize total taxes collected while minimizing the impact of taxation on the population over a finite time. Solutions to the optimal control problem yield taxation rates specific to an agent's location and current wealth. The use of optimal controls (generated by the PDE model) within the ABM performed better than other controls we evaluated, even though some error was introduced between the ABM and PDE models.

Rachael Miller Neilan
Duquesne University
rachael.neilan@gmail.com

Scott Christley
University of Texas Southwestern Medical Center
scott.christley@utsouthwestern.edu

Matthew Oremland
Mathematical Biosciences Institute
Ohio State University
oremland.2@mbi.osu.edu

Rene Salinas
Appalachian State University
salinasra@appstate.edu

Suzanne M. Lenhart
University of Tennessee
Department of Mathematics
lenhart@math.utk.edu

MS37
Optimal Control Applied to an Anthrax Outbreak Model for Wild Animals

Anthrax is a fatal disease common to many wild animals especially herbivore mammals. It is endemic to several national parks and one of the main causes of herbivore decline. Most anthrax infected animals face inevitable death and each infected carcass deposits massive number of spores into the surrounding environment. Infected animals and infected carcasses are considered to be the main sources of new infections. Thus, controlling new infections through vaccination and eliminating spread through proper carcass disposal are the only feasible ways to effectively control the disease when an outbreak occurs. In this talk, a system made up of parabolic partial differential equations together with ordinary differential equations will be presented and effect of the two most commonly used controls on disease transmission will be investigated. Some numerical results will also be presented.

Buddhi Pantha
Department of Mathematics
University of Tennessee
bpantha@utk.edu

Suzanne M. Lenhart
University of Tennessee
Department of Mathematics
lenhart@math.utk.edu

Judy Day
University of Tennessee
judyday@utk.edu

MS38
Systems, Generativity and Interactional Effects

Our principal concern is to understand and uncover interaction-related effects that arise from the interaction of systems. We may describe the situation of interest as systems coming together, interacting and producing as an aggregate a behavior that would not have occurred without interaction. Those situations are fundamental and appear in countless settings, such as those exhibiting cascade-like intuition. The goal is to show that one can extract from a system the potential it has to generate such effects, and use those extracts to reconstruct, or characterize, the phenomena that emerge upon interaction. We propose a means to relate properties of an interconnected system to its separate component systems in the presence of cascade-like effects. Building on a theory of interconnection reminiscent of the behavioral approach to systems theory, we introduce the notion of generativity and its byproduct, generative effects. Cascade effects are seen as instances of generative effects. The latter are the instances where properties of interest are not preserved or behave badly when systems interact. The work overcomes that obstruction. We show how to extract algebraic objects from the systems that encode their generativity: their potential to generate new phenomena upon interaction. Those objects may then be used to link the properties of the interconnected system to its separate systems. Such a link will be executed through the use of exact sequences from commutative algebra.

Elie Adam
MIT
eadam@mit.edu

MS38
Sheaves over Networks for Inference

In this talk, I'll argue that the recent advances in applied algebraic topology point to cellular sheaves as good structures for modelling data tethered to spaces; and cohomology as an especially useful compression of such data. I'll focus on one example in pursuit-evasion and tracking, closing with how computational issues arise and are addressed with novel mathematical perspectives.

Robert W. Ghrist
University of Pennsylvania
ghrist@seas.upenn.edu

MS38
A Sheaf Theoretic Modeling and Compositional Framework for Complex SoS

To achieve a scalable design paradigm most of complex systems are developed by first designing, analyzing and testing subsystems and then by interconnecting them. In order to achieve scalability without completely sacrificing analytical guarantees one needs to mathematically formalize the composition operation. One of the key characteristics such a framework needs to have is the ability to easily compose different models of computation. These are conveniently used to design and analyze each subsystem, but such model may become extremely inconvenient at the time of the composition. This means that the designer needs to first choose a common abstraction model and then translate each submodel in order to compose. In this talk we discuss a new framework for modeling and composing system of systems. The framework enables us to translate various mathematical submodels into a common abstraction based on *interval sheaves*. Leveraging the compositionality properties of sheaves we are able to define abstract machines that can be composed in an arbitrary way with strong mathematical guarantees. We introduce this framework and then show its applicability to an aerospace scenario. While the example is fairly simple, the purpose is to highlight the capability of the sheaf-based abstraction to enable composition of subsystems that are inherently described by very different models of computation.

Alberto Speranzon
Honeywell Aerospace
alberto.speranzon@gmail.com

MS38
Compositional Contracts for Hybrid Dynamical Systems

We consider a very general type of machine that includes discrete, continuous, or quite generally "hybrid" systems. Such machines can be wired together to compositionally form larger-scale machines, either statically or dynamically in time. We will discuss a language in which to specify contracts – behavioral guarantees – for such machines, and give a composition operation on contracts that corresponds to the composition operation for machines.

David I. Spivak
MIT
dspivak@mit.edu

MS39
Bilevel NLP Formulations for Singular Optimal Control Problems

Singular optimal control problems arise frequently on a broad range of chemical engineering applications. Determination of the accurate dynamic structure of the optimal solution profile and the junctions between optimal nonsingular and singular arcs is essential for operating strategies, as well as equipment designs for many processes. In a previous study (Chen, Shao and Biegler, AIChE J 2014) we developed a nested optimization formulation that finds the optimal mesh distribution and determines exact control profiles for nonsingular optimal control problems without state constraints. This study extends this approach to singular optimal control problems. To satisfy the necessary optimality conditions for singular optimal control problems with a well-defined solution strategy, the overall nonlinear programming formulation resulting from direct transcription is decomposed into inner and outer problems. The key feature of this algorithm is that it converges to a solution that satisfies the discretized Euler-Lagrange equations of the original singular optimal control problem; we prove this under suitable assumptions. This is obtained through the introduction of pseudo-multipliers that reconstruct the necessary optimality conditions for singular optimal control in the outer problem. We demonstrate this approach on eight classical singular control problems with known so-

lutions, as well as three larger singular control problems derived from chemical engineering applications.

Weifeng Chen
Zhejiang University of Techology
wfchen@zjut.edu.cn

Lorenz T. Biegler
Carnegie Mellon University
Pittsburgh, USA
biegler@cmu.edu

MS39
A Multi-scale Decomposition Strategy for Concentrated Solar Power Systems

As energy markets and infrastructures continue to evolve, large electricity consumers and generators are seeking new ways to increase revenues by responding to time-varying energy prices. For large-scale concentrated solar power (CSP) systems, operational flexibility comes from thermal energy storage. In this talk, we present a mathematical model for CSP systems and pose multi-scale electricity market participation as a non-convex mixed integer nonlinear programming. We discuss computational challenges for existing solvers (e.g., SCIP) and propose a multiscale decomposition algorithm. Discrete decisions such as equipment modes are determined in a scheduling problem (MILP) with a coarse (1-hour) time discretization. CSP system physics are simplified by decoupling mass and energy balances. Next, full resolution system physics are considered in a nonlinear dynamic optimization problem (NLP) using direct transcription with 5-minute time intervals and fixed discrete decisions. The results, including a high-resolution enthalpy profile, are used to update the simplified model in the scheduling problem for the next iteration. Using this approach, we find the potential increase revenues by 10-25% and 100% through participation in ancillary service and real-time energy markets, respectively. These revenues require fast flexibility (order minutes) and thus were missed in previous analyses that focused only on day-ahead markets (1-hour intervals).

Alexander W. Dowling
University of Wisconsin-Madison
Department of Chemical and Biological Engineering
adowling2@wisc.edu

Victor Zavala
University of Wisconsin-Madison
victor.zavala@wisc.edu

MS39
Generalized Derivatives of Nonlinear Programs for use in Model Predictive Control

Parametric sensitivities are obtained for NLPs exhibiting active set changes. The sensitivity system found is a nonsmooth and nonlinear equation system that characterizes primal and dual sensitivities as its unique solution and recovers the classical results of Fiacco and McCormick in the absence of active set changes. Built using Nesterovs lexicographic differentiation, a new tool in nonsmooth analysis called the lexicographic directional derivative is used to evaluate generalized derivative elements of NLPs. The generalized derivative information is furnished under regularity conditions implied by, for example, a KKT point satisfying LICQ and strong second-order sufficiency. The nonsmooth and nonlinear sensitivity system can be solved

in a tractable way to characterize computationally-relevant generalized derivative elements of NLPs. Application to nonlinear model predictive control acts as motivation to this work.

Peter G. Stechlinski
Process Systems Engineering Laboratory
Massachusetts Institute of Technology
pstechli@mit.edu

Johannes Jaschke
Department of Chemical Engineering
Norwegian University of Science and Technology
johannes.jaschke@ntnu.no

Kamil Khan
Massachusetts Institute of Technology
Department of Chemical Engineering
kamil@alum.mit.edu

Paul I Barton
Process Systems Engineering Laboratory
Massachusetts Institute of Technology
pib@mit.edu

MS39
Optimization Formulations for Robust Nonlinear Model Predictive Control

Model Predictive Control (MPC) has been widely used in process control industry mainly because it can deal with constraints and multiple-input-multiple-output. However, the system performance deteriorates under the influence of uncertainty. The current robust MPC techniques are often shy of applications due to either model conservativeness or formidable computational effort. In order to improve this situation, this talk presents a multistage nonlinear model predictive control (NMPC) framework to serve as a promising non-conservative robust NMPC scheme. Multistage NMPC models the uncertainty evolution with a truncated scenario tree whose structure exploits the degrees of freedom by allowing future control inputs to adjust to future available information. A nonlinear CSTR example with a setpoint tracking objective has been explored with two separate uncertain parameters: activation energy and inlet concentration. Under both cases, the performance of multistage NMPC is superior than standard NMPC and other robust NMPC approaches, such as min-max NMPC and robust NMPC with backoff constraints, where backoff terms are calculated from Monte Carlo simulations. Also, multistage scheme of different number of robust horizons is investigated and results are discussed. Lastly, a sensitivity-based path-following algorithm has been developed for multistage NMPC models, to achieve a computational effort comparable with nominal dynamic optimization problem.

Zhou (Joyce) Yu
Carnegie Mellon University
zhouy1@andrew.cmu.edu

Lorenz T. Biegler
Carnegie Mellon University
Pittsburgh, USA
biegler@cmu.edu

MS40
On the Feedback Stabilization to Trajectories for

Semilinear Parabolic Equations

Recent results on the feedback stabilization to trajectories for parabolic equations by means of a finite number of actuators are presented. After linearization around the targeted time-dependent trajectory one has to deal with the stabilization of a nonautonomous linear parabolic equation. Dealing with the nonautonomous case requires tools different from the spectral properties used to deal with the autonomous one. Both internal and boundary actuators will be considered.

Sergio Rodriguez
Johann Radon Institute for Computational and
Applied Mathematics
sergio.rodrigues@oeaw.ac.at

MS40

Numerical Simulations for the Control and Estimation of the 2D Burgers Equation

A numerical approach for the local stabilization of Burgers equation, based on boundary feedback control and boundary observation, is presented. This requires coupling the system with an estimator in order to obtain a compensated system [J.P. Raymond, J.M. Buchot, J. Tiago, Coupling estimation and control for a two dimensional Burgers type equation, ESAIM-COCV, Vol 21, Number 2, pp. 535-560 (2015)]. Simulations in different domains related to idealized cardiovascular geometries are presented to validate the method [J. Tiago, Numerical simulations for the stabilization and estimation problem of a semilinear partial differential equation, Appl. Numer. Math., Vol. 98, pp. 18-37 (2015)].

Jorge Tiago
CEMAT, Instituto Superior Tecnico, Universidade de
Lisboa
jftiago@math.tecnico.ulisboa.pt

Jean Pierre Raymond
Institut de mathematique, UPS
Toulouse, France
jean-pierre.raymond@math.univ-toulouse.fr

Jean-Marie Buchot
Institut de Mathématiques de Toulouse, France
jean-marie.buchot@math.univ-toulouse.fr

MS40

Optimal Control of the Stochastic Navier-Stokes Equation with Lévy Noise

We consider an optimal control problem for incompressible flows governed by the stochastic Navier-Stokes equation in a multidimensional domain with jumps occurring in the noise term. The control problem introduced in this talk is motivated by common strategies, such as tracking a desired state and minimizing the enstrophy energy. Since the existence and uniqueness of a mild solution is provided only locally in time, the cost functional has to incorporate a stopping time, which depends on the control. We show that the cost functional is continuous with respect to the controls, and this enables us to prove the existence and uniqueness of the optimal control. Necessary and sufficient optimality conditions are derived based on the Fréchet derivative of the control-to-state mapping as the solution of the linearized stochastic Navier-Stokes equation. Hence, we can conclude that the stochastic optimal controls satisfy a feedback law.

Christoph Trautwein
Max Planck Institute
trautwein@mpi-magdeburg.mpg.de

Peter Benner
Max Planck Institute for Dynamics of Complex Technical
Systems, Magdeburg, Germany
benner@mpi-magdeburg.mpg.de

MS41

Fractional Operators with Inhomogeneous Boundary Conditions: Analysis, Control, and Discretization

In this talk we introduce new characterizations of spectral fractional Laplacian to incorporate nonhomogeneous Dirichlet and Neumann boundary conditions. The classical cases with homogeneous boundary conditions arise as a special case. We apply our definition to fractional elliptic equations of order $s \in (0,1)$ with nonzero Dirichlet and Neumann boundary conditions. Here the domain Ω is assumed to be a bounded, quasi-convex Lipschitz domain. To impose the nonzero boundary conditions, we construct fractional harmonic extensions of the boundary data. It is shown that solving for the fractional harmonic extension is equivalent to solving for the standard harmonic extension in the very-weak form. The latter result is of independent interest as well. The remaining fractional elliptic problem (with homogeneous boundary data) can be realized using the existing techniques. We introduce finite element discretizations and derive discretization error estimates in natural norms, which are confirmed by numerical experiments. We also apply our characterizations to Dirichlet and Neumann boundary optimal control problems with fractional elliptic equation as constraints.

Harbir Antil
George Mason University
Fairfax, VA
hantil@gmu.edu

Johannes Pfefferer
Technische Universität München
Zentrum Mathematik
pfefferer@ma.tum.de

Sergejs Rogovs
Department of Mathematics
University of Bundeswehr Munich
sergejs.rogovs@unibw.de

MS41

A Coupling Strategy for Nonlocal and Local Models with Applications to Static Peridynamics

The use of nonlocal models in science and engineering applications has been steadily increasing over the past decade. The ability of nonlocal theories to accurately capture effects that are difficult or impossible to represent by PDEs motivates the interest in these simulations. However, the accuracy of nonlocal models comes at the price of an increase in computational costs. Thus, it is important to develop coupling strategies that aim to combine the accuracy of nonlocal models with the computational efficiency of PDEs. The basic idea is to use the more efficient PDE model everywhere except in those parts of the domain that require the improved accuracy of the nonlocal model. We

develop and analyze an optimization-based method for the coupling of nonlocal and local problems. The approach is formulated as a control problem where the states are the solutions of the nonlocal and local equations, the objective is to minimize their mismatch on the overlap of the nonlocal and local domains, and the controls are virtual volume constraints and boundary conditions. We prove that the resulting optimization problem is well-posed and discuss its implementation. Numerical results in three-dimensions illustrate key properties of the optimization-based coupling method; these numerical tests provide the groundwork for the development of efficient and effective engineering analysis tools. As an application, we present results for a static peridynamic model.

Marta D'Elia
Sandia National Laboratories
mdelia@sandia.gov

Pavel Bochev
Sandia National Laboratories
Computational Math and Algorithms
pbboche@sandia.gov

David Littlewood
Sandia National Laboratories
djlittl@sandia.gov

Mauro Perego
CSRI Sandia National Laboratories
mperego@sandia.gov

MS41

High-performance Computing for Optimal Control of Fractional Partial Differential Equations

In recent years nonlocal operators, especially the fractional Laplacian, have received much attention both in pure and in applied mathematics. Among other applications, these operators emerge in nonlocal diffusion models which arise in fields where the phenomena cannot be described accurately by standard diffusion models. There are a variety of such applications, including phase transitions, image analysis or nonlocal heat conduction. We are interested in PDEs involving the fractional Laplacian using the spectral definition and its extension to fractional powers of general second order elliptic operators. Several numerical methods have been developed to solve these problems, such as spectral methods, the matrix transference technique (MTT), or FEM. Spectral methods and MTT require the solution of a large number of eigenvalue problems. Finite element methods are based on the extension approach by Caffarelli and Silvestre. This approach allows to localize the nonlocal problem but comes at the expense of incorporating an additional space dimension to the problem. For all methods, it is indispensable to develop efficient numerical algorithms to deal with the nonlocality of the operator. We will consider optimal control problems governed by fractional partial differential equations and use FEM to solve the PDEs. To handle the computational effort involved, we investigate numerical algorithms for the solution of fractional PDEs on parallel computers.

Dominick Gallo, Martin Siebenborn
University of Trier
DFG-RTG Algorithmic Optimization
gallo@uni-trier.de, siebenborn@uni-trier.de

MS41

Optimal Control for Nonlocal Elliptic Problems in Three Dimensions

Our aim is to control the source term of general nonlocal volume constrained diffusion problems with the means of optimal control methods. The theoretical foundation of our talk is the recently formulated nonlocal finite element framework by Max Gunzburger et al. allowing for a numerical treatment of general nonlocal diffusion problems. The nonlocal elliptic operator studied in these works include for example the integral definition of the fractional Laplace operator as a special case. Due to nonlocal interactions and possibly singular kernel functions, this becomes a numerically challenging task when going beyond preliminary examples in one dimension. Our approach is to consider translationally invariant kernel functions which allow us to implement an efficient algorithm for solving the above mentioned control problem on a structured grid in three dimensions.

Volker H. Schulz
University of Trier
Department of Mathematics
Volker.Schulz@uni-trier.de

Christian Vollmann
University of Trier
DFG-RTG Algorithmic Optimization
vollmann@uni-trier.de

MS42

Control in the Singular Perturbations Limit

We examine the form the controls and optimal controls in the limit of general singularly perturbed systems take, and the relations with the optimal controls of the perturbed systems. We do not assume that an amenable order reduction limit is available, thus, the limit in the general case utilizes probability measure-valued dynamics which may depend on slow observables.

Zvi Artstein
The Weizmann Institute of Science
zvi.artstein@weizmann.ac.il

MS42

From the Divergence Theorem to Occupational Measures and Infinite-horizon Optimization

We present new tight bounds for flux integrals, which we use to characterise singular limits of occupational measures. This characterization is then applied to several singular optimization problems: planar infinite-horizon optimal control, planar Cheeger set and generalized Cheeger set, and higher dimensional shape optimization problems.

Ido Bright
University of Washington
ibright@ebay.com

MS42

On the Euler Equation and the Transversality Con-

dition of Macroeconomic Dynamics

In this talk, we consider the traditional capital accumulation model with continuous time, and derive the Euler equation for a necessary condition and the Euler equation with the transversality condition for a sufficient condition of overtaking (or, weakly overtaking) optimality. In addition, we try to solve this model with AK technology, and show both that the necessary and sufficient condition of the existence of overtaking optimal solution and that the form of this solution. In particular, we solve the case in which the utility function is CRRA, and show that this solution has a finite value.

Yuhki Hosoya
Department of Economics
Kanto-Gakuin University
hosoya@kanto-gakuin.ac.jp

MS42

Recursive Variational Problems in Nonreflexive Banach Spaces with an Infinite Horizon: An Existence Result

We investigate convex variational problems with recursive integral functionals governed by infinite-dimensional differential inclusions with an infinite horizon and present an existence result in the setting of nonreflexive Banach spaces. We find an optimal solution in a Sobolev space taking values in a Banach space such that the derivatives are Bochner integrable functions. We also investigate sufficient conditions for the existence of solutions to the initial value problem for the differential inclusion.

Nobusumi Sagara
Department of Economics
Hosei University
nsagara@hosei.ac.jp

MS43

Reduced Order Filtering Algorithms

We develop reduced order filtering algorithms for a general class of nonlinear PDE model dynamics. It is based on the projected Gaussian filter and reduced order method by the singular value decomposition of the error covariance. We develop a direct update of square root factors for the covariance. It works very effectively with a small number of sampling directions as a collection singular vectors and captures the essential dynamics of the filtering dynamics. Stability and convergence analysis of algorithms are presented along with numerical test examples.

Kazufumi Ito
North Carolina State University
kito@ncsu.edu

MS43

A Sparse-grid UKF For the State Estimation of PDEs

Unscented Kalman Filter (UKF) has been widely used in the estimation of dynamical systems defined by ordinary differential equations. For partial differential equations, their discretized systems often have very high dimensions, which result in covariance matrices that are computationally intractable. In this paper, we introduce sparse-grids and an associated reduced state space, called a surplus space, in which the covariance matrices have relatively small dimensions and the number of sigma points is significantly reduced. The covariance in the reduced space can be used to compute the correction term for the updating process of the UKF. The resulting sparse-grid UKF is illustrated using an example of shallow water equations.

Wei Kang
Naval Postgraduate School
Department of Applied Mathematics
wkang@nps.edu

Sarah King, Liang Xu
Naval Research Laboratory
sarah.king@nrlmry.navy.mil, liang.xu@nrlmry.navy.mil

MS43

DMD-based Estimation of the Flow Field behind a Thin Airfoil at High Angles of Attack by Assimilating Distributed Pressure Measurements

Recent advances in Dynamic Mode Decomposition (DMD) and Koopman operator theory approaches to nonlinear systems have revealed that nonlinear dynamics can be linearly encoded using Koopman eigenfunctions and Koopman modes (or similarly, the modes of dynamic mode decomposition from the fluids literature). Taking a subset of these dynamic modes provides a reduced-order, linear model of the system dynamics without linearization. The DMD modes can be used to achieve realistic and computationally inexpensive estimates of the flow field. We construct a reduced-order model of the flow past an airfoil operating at a high angle of attack through computational fluid dynamics (CFD) simulations. We implement a Kalman filter using the reduced-order model to estimate the state of the flow velocity field using measurements from a distributed array of pressure sensors.

Frank D. Lagor
University of Maryland
Department of Aerospace Engineering
flagor@umd.edu

Derek A. Paley
University of Maryland
Dept. Aerospace Engineering and Inst. for Systems
Research
dpaley@umd.edu

MS43

Disturbance Estimation of a Wave PDE on a Time-varying Domain

In this paper, we design an exponentially convergent disturbance observer for a wave PDE on a time-varying domain by using two boundary measurements $u(0, t), u_t(l(t), t)$. More specifically, two PDEs are constructed to build the disturbance observer for tracking the external disturbance in the wave PDE. Exponential convergence of the disturbance estimation to the true disturbance value is proved by Lyapunov analysis, with which all states in the observer are shown to be bounded. This method can be used in many industrial applications such as mining cable elevators.

Ji Wang
State Key Laboratory of Mechanical Transmission
Chongqing University, China
wangji@cqu.edu.cn

Shuxia Tang
Department of Mechanical and Aerospace Engineering
University of California San Diego
shuxiatang.control@gmail.com

Yangjun Pi
State Key Laboratory of Mechanical Transmission
Chongqing University, China
cqpp@cqu.edu.cn

Miroslav Krstic
University of California, San Diego
Dept of Mechanical & Aerospace Engineering
krstic@ucsd.edu

MS44

Connection Between MP and DPP for Stochastic Recursive Optimal Control Problems

This talk deals with a stochastic recursive optimal control problem, where the diffusion coefficient depends on the control variable and the control domain is not necessarily convex. After some review of classical results in the literatures, we focus on the connection between the general maximum principle and the dynamic programming principle for such control problem without the assumption that the value is smooth enough, the set inclusions among the sub- and super-jets of the value function and the first-order and second-order adjoint processes as well as the generalized Hamiltonian function are established. Moreover, by comparing these results with the classical ones in J. Yong and X. Zhou [Stochastic Controls: Hamiltonian Systems and HJB Equations, Springer-Verlag, New York, 1999], it is natural to obtain the first- and second-order adjoint equations of M. Hu [Stochastic global maximum principle for optimization with recursive utilities, Probability, Uncertainty and Quantitative Risk, Vol. 2, Article 1, 20 pages, 2017].

Tianyang Nie, Jingtao Shi
School of Mathematics
Shandong University
nietianyang@sdu.edu.cn, shijingtao@sdu.edu.cn

Zhen Wu
Shandong University, China
wuzhen@sdu.edu.cn

MS44

Some Results on Optimal Stopping Problems for One-dimensional Regular Diffusions

For a class of optimal stopping problems, we provide a complete characterization for optimal stopping/continuation regions. Some comparison principles for critical levels and value functions are also given. The key tool is the characterization of the value functions for general one-dimensional regular diffusion processes developed by Savas Dayanik and Ioannis Karatzas in 2003. This is a joint work with Dongchao Huang.

Jian Song, Dongchao Huang
The University of Hong Kong
txjsong@hku.hk, huangdongchao2012@gmail.com

MS44

An Implicit Numerical Scheme for a Class of Back-ward Doubly Stochastic Differential Equations

In this paper, we consider a class of backward doubly stochastic differential equations (BDSDE for short) with general terminal value and general random generator. Those BDSDEs do not involve any forward diffusion processes. By using the techniques of Malliavin calculus, we are able to establish the L^p-Hölder continuity of the solution pair. Then, an implicit numerical scheme for the BDSDE is proposed and the rate of convergence is obtained in the L^p-sense. As a by-product, we obtain an explicit representation of the process Y in the solution pair to a linear BDSDE with random coefficients.

Xiaoming Song
Department of Mathematics
Drexel University
song@math.drexel.edu

Yaozhong Hu, David Nualart
Department of Mathematics
University of Kansas
yhu@ku.edu, nulart@ku.edu

MS44

A Stochastic Maximum Principle for Processes Driven by G-Brownian Motion and Applications to Finance

Based on the theory of stochastic differential equations on a sublinear expectation space $(\Omega, \mathcal{H}, \hat{\mathbb{E}})$, we develop a stochastic maximum principle for a general stochastic optimal control problem, where the controlled state process is a stochastic differential equation driven by G-Brownian motion. Furthermore, under some convexity assumptions, we obtain sufficient conditions for the optimality of the maximum in terms of the $\mathcal{H}$-function. Finally, applications of the stochastic maximum principle to the mean-variance portfolio selection problem in the financial market with ambiguous volatility is discussed.

Zhongyang Sun
School of Mathematics
Sun Yat-sen University
zysun
_nk@126.com

Xin Zhang
Department of Mathematics
Southeast University
x.zhang.seu@gmail.com

Junyi Guo
School of Mathematical Sciences
Nankai University
jyguo@nankai.edu.cn

MS45

Are American Options European after all?

This talk addresses one of the fundamental problems in mathematical finance: pricing of American type options. Here, American type means that the holder has the right to exercise the option at any time point up to a pre-specified maturity time. Although the underlying theory is discussed in every introductory textbook, both the mathematical and applied treatment is challenging even in unrealistically simplified models such as a standard Black Scholes model. This is a fundamental difference to European style

options. In this talk we discuss the question whether the value of an American option actually coincides in the continuation region with that of a properly chosen European payoff. In analytical terms this boils down to the question whether a harmonic function solving a free boundary problem can be extended to a harmonic function on the whole space. In cases where the answer is positive, this opens the door for very efficient new methods for treating American options for both theory and practice. The talk is mainly based on Christensen (2014) [Mathematical Finance 24, 156-172] and Christensen, Kallsen, Lenga (2016).

Soren Christensen
University of Hamburg, Germany
soeren.christensen@uni-hamburg.de

MS45

Infinite-horizon Non-zero-sum Stochastic Differential Games with Additive Structure

This talk deals with infinite-horizon non-zero-sum stochastic differential games with discounted and average payoffs and an additive structure. The objective is to show conditions for the existence of Nash equilibria in the set of stationary randomized strategies for the discounted payoff and then, by following the vanishing discount approach, to show the existence of Nash equilibria for the average payoff. To this end, we will use standard dynamic programming techniques.

Hector Jasso-Fuentes
CINVESTAV-IPN
hjasso@math.cinvestav.mx

B. Adriana Escobedo-Trujillo
Civil Engineering Faculty. Universidad Veracruzana
Mexico
bescobedo@uv.mx.

J. Daniel Lopez-Barrientos
Faculty of Actuarial Sciences
Faculty of Actuarial Sciences, Universidad Anahuac Norte
daniel.lopez@anahuac.mx

MS45

Optimal Asset Allocation with Stochastic Interest Rates in Regime-switching Models

In this talk we present some results on optimal asset allocation with stochastic interest rates in Markovian regime-switching models. A power utility function is considered. When a regime-switching Vasicek model is assumed for the interest rate, a closed-form solution is obtained. When a regime-switching CIR model is assumed for the interest rate, a numerical algorithm is developed to solve the associated system of nonlinear PDEs. A verification argument is provided.

Cheng Ye
University of Dayton
yec003@udayton.edu

Ruihua Liu
University of Dayton
Department of Mathematics
rliu01@udayton.edu

Dan Ren, Muhammad Usman

University of Dayton
dren01@udayton.edu, musman1@udayton.edu

MS45

Optimal Consumption and Investment on a Finite Horizon

This paper considers a utility of spending scaled by the past peak spending, and solves an optimal spending-investment problem on a finite horizon. A closed form solution suggests that the spending rate is constant and equals the historical peak for relatively large values of wealth/peak consumption, decreases when the ratio is relatively small, and in particular, increases when the ratio reaches an upper bound.

Dan Ren
University of Dayton
dren01@udayton.edu

MS46

Discontinuous Solutions of Hamilton-Jacobi Equations on Networks

In the paper presented, we study optimal control problems on networks without controllability assumptions at the junctions. The Value Function associated with the control problem is characterized as the solution to a system of Hamilton-Jacobi equations with appropriate junction conditions. The novel feature of the result lies in that the controllability conditions are not needed and the characterization remains valid even when the Value Function is not continuous.

P. Jameson Graber
Baylor University
jameson_graber@baylor.edu

Cristopher Hermosilla
ENSTA ParisTech
cristopher.hermosilla@polytechnique.edu

Hasnaa Zidani
ENSTA ParisTech, INRIA Saclay
hasnaa.zidani@ensta-paristech.fr

MS46

Optimal Open-loop Strategies in a Debt Management Problem

We study optimal strategies for a borrower who needs to repay his debt, in an infinite time horizon. An instantaneous bankruptcy risk is present, which increases with the size of the debt. This induces a pool of risk-neutral lenders to charge a higher interest rate, to compensate for the possible loss of part of their investment. Solutions are interpreted as Stackelberg equilibria, where the borrower announces his repayment strategy $u(t)$ at all future times, and lenders adjust the interest rate accordingly. This yields a highly nonstandard problem of optimal control, where the instantaneous dynamics depends on the entire future evolution of the system. Our analysis shows the existence of optimal open-loop controls, deriving necessary conditions for optimality and characterizing possible asymptotic limits as $t \to +\infty$.

Yilun Jiang
Penn State University

yxj141@psu.edu

Alberto Bressan
Pennsylvania State University
bressan@math.psu.edu

MS46

Growth Model for Tree Stems and Vines

In this talk, we propose a model describing the growth of tree stems and vine, taking into account also the presence of external obstacles. The system evolution is described by an integral differential equation which becomes discontinuous when the stem hits the obstacle. The stem feeling the obstacle reaction not just at the tip, but along the whole stem represents one of the main challenges. Indeed, this produces a cone of possible reactions which is not normal with respect to the obstacle and affects the whole stem. However, using tools from geometry and optimal control, we are still able to prove existence and uniqueness of the solution under natural assumptions on the initial data.

Michele Palladino
Penn State University
mup26@psu.edu

Alberto Bressan
Pennsylvania State University
bressan@math.psu.edu

Wen Shen
Penn State University
shen_w@math.psu.edu

MS46

On the Stability Property for Time-delayed Differential Inclusions

This talk addresses the issue upon the stability property for a time-delayed system parametrized by a differential inclusion. We announce sufficient conditions of Lyapunov type for the most pedestrian notions of stability when the dynamics under consideration is discontinuous, multivalued, and exhibits a time delay component that features under very mild hypotheses.

Vinicio Rios
Universidad del Zulia
Maracaibo, Venezuela
vrios@demat-fecluz.org

MS47

Categorical Perspectives on Hybrid Systems with a View toward Robotics

In this talk I will discuss about hierarchical representations in hybrid systems, systems of hybrid systems through the small category/functor representation of hybrid objects over a category. In particular, I will discuss how this relates to model category theory, and connect this with real life examples on robotics systems.

Aaron D. Ames
Department of Mechanical Engineering
Texas A&M University
ames@caltech.edu

MS47

A Mathematical Theory of Co-design

I will describe a mathematical theory of co-design. The objects of this theory are design problems, described as feasibility relations between functionality provided and resources used. The basic property studied is a monotonicity property, which is: if the required functionality is increased, the required resources do not decrease. This property is intrinsic, in the sense that is invariant to any order-preserving reparameterization. I will show that this family of Monotone Co-Design Problems (MCDPs) is closed to composition operations through operations that are the equivalent of series, parallel, and feedback interconnection. The queries that can be answered based on these models are of the form minimize resources, subject to minimal functionality provided or, dually, maximize functionality, subject to maximum resources usage. I will show that weak assumptions of monotonicity are sufficient to allow a systematic solution procedure that finds the set of all non-dominating solutions based on the elementary theory of fixed points on partially ordered sets (Kleene/Tarski). The complexity depends on the richness of the functionality/resources spaces (measured by height and width of their posets), as well as the structure of the co-design graph. I will also describe a formal language for describing MCDPs as well as a prototype interpreter/solver. Open-source software is available at http://mcdp.mit.edu/.

Andrea Censi
MIT
censi@mit.edu

MS47

When is the Interconnection of Controllable Systems Controllable?

I will present some preliminary results on this problem for linear discrete-time time-invariant (LTI) dynamical systems. These, and their controllability, will be defined in the sense of Willems. Our approach will be category theoretic, resulting in a sound and complete graphical theory for reasoning about the equivalence of LTI systems. This graphical syntax turns out to be closely related to the classical notion of signal flow diagrams.

Brendan Fong
University Of Pennsylvania
fo@seas.upenn.edu

MS47

Exploiting Structure in the Construction of Finite-state Abstractions of Control Systems

Finite-state abstractions of differential equations modeling control systems have successfully been used to synthesize controllers enforcing complex specifications such as those expressed in temporal logic. Unfortunately, the construction of these abstractions suffers from the infamous curse of dimensionality. In this talk I will describe how one can exploit the structure of the differential equations modeling control systems to construct finite-state abstractions compositionally, thereby taming the curse of dimensionality. Starting from a concrete example of structure, partial feedback linearizability, I will employ basic ideas of cate-

gory theory to move towards a general theory.

Paulo Tabuada
Dept. of Electrical Engineerin
Univ. of California, Los Angel
tabuada@ee.ucla.edu

MS48

Real-Time Feasible Online Computation of Constrained Nonlinear Optimal Feedback

NMPC - Nonlinear Model Predictive Control - is probably one of todays most promising approaches to constrained optimal feedback control of nonlinear processes under uncertainties. Its basic idea is to use a sufficiently detailed nonlinear dynamical model to predict the performance of the process to be controlled over a suitably long time horizon. To cope with perturbations an optimal feedback control is then computed by frequent online solution of the corresponding optimal control problem subject to equality and inequality constraints. A major numerical challenge is to speed up these computations such that the approach is real-time feasible also for fast processes and complex models as, e.g., in vehicle dynamics. The presentation will outline some of the algorithmic ideas involved in the so called multi-level real-time iterations and the online active set strategy in particular, which have produced a speed-up by 4 5 orders of magnitude over earlier approaches to NMPC. Extensions to mixed-integer optimal feedback control will be sketched and applications to engineering problems such as energy conservation in heavy duty trucks will be given.

Hans Georg Bock
IWR, University of Heidelberg
bock@iwr.uni-heidelberg.de

MS48

Optimal Feedback Control for Average Output Systems

In this talk we consider the class of average output optimal control problems (AOCPs) and feedback control for such systems. AOCPs are characterized by long (also infinitely long) time horizons and an objective criterion which, on the long time horizon, can only be evaluated in an averaged sense (e.g. energy output of pumped storage hydroelectric plant). Such problems arise naturally for example in the energy sector or in chemical process industry. AOCPs are numerically hard to solve because of the long time horizon, especially if the objective is of economic type. This makes optimal feedback control for such systems challenging. We present a method that is based on the fact that an AOCP can be approximated arbitrarily well by an optimal control problem on a finite time horizon with an additional periodicity constraint. This approach allows us to significantly reduce the computational effort, which makes AOCPs accesible to optimal feedback control. Finally a numerical case study we apply our method to the example of a power generating flying kite.

Juergen Gutekunst
IWR, University of Heidelberg
juergen.gutekunst@iwr.uni-heidelberg.de

Andreas Potschka
Interdisciplinary Center for Scientific Computing
University of Heidelberg
potschka@iwr.uni-heidelberg.de

Hans Georg Bock
IWR, University of Heidelberg
bock@iwr.uni-heidelberg.de

MS48

Nonlinear Optimal Feedback Control for Wine Fermentation by Economic NMPC

In the process of making wine a high potential for the conservation of energy exists. That is why minimizing the energy needed for cooling during wine fermentation plays a significant role. Therefore, we study nonlinear optimal feedback control of the cooling process during wine fermentation by using economic nonlinear model predictive control (ENMPC). We discuss especially the numerical challenges arising from this context.
Thereby, a solution strategy for nonlinear control problems with changing model parameters, unknown disturbance factors and changes in the states is introduced. The objective is a combination of an economic type and a tracking type objective considering the minimization of energy but also maintaining the quality of the white wine. Moreover, the parameters and states determining the fermentation dynamics are consistently estimated from measurements and the optimal cooling profile is computed and adjusted.
The process of wine fermentation is described by a novel model including a death phase for yeast and the influence of oxygen on the process. This model is solved numerically using collocation methods for the discretization of the time-dependent differential equations and the control. Optimization is performed using Pyomo for the formulation of the optimization problem and IPOPT for its solution.
The numerical results for this ENMPC controller and a traditional controller are compared and discussed.

Christina Schenk
University of Trier
christina.schenk@uni-trier.de

Volker H. Schulz
University of Trier
Department of Mathematics
Volker.Schulz@uni-trier.de

MS48

Economic Nonlinear Model Predictive Control (NMPC) for CO2 Capture Systems

We describe a framework for Nonlinear Model Predictive Control of large-scale DAE systems using direct transcription for dynamic optimization, along with a flexible, uniform environment to manage the optimization and data transfer. For this, the Pyomo platform implements all NMPC tasks such as model discretization and optimization in a single platform. Our target application is the solid sorbent based adsorption process, a promising approach for CO2 capture in power plants. In this system, bubbling fluidized beds (BFBs) enable efficient gas-solid contact and heat transfer. Consequently, optimal operation of the BFB reactors require efficient controllers that keep the system within the environmental and safety constraints. The BFB model consists of a large-scale nonlinear system of partial-differential algebraic equations which include mass and energy balances, coupled with correlations for hydrodynamics and thermodynamic properties. This model can provide an accurate description of the behavior of the process, but its implementation in control is limited because of the computational cost involved. To overcome

this barrier, we apply a sensitivity-based advanced step NMPC algorithm, which moves the expensive dynamic optimization problem offline and enables fast online control. Moreover, in addition to setpoint tracking and disturbance rejection capabilities, our proposed NMPC framework can directly optimize process economic performance within the control loop.

David Thierry, Mingzhao Yu
Carnegie Mellon University
dmolinat@andrew.cmu.edu, mingzhaoyu@cmu.edu

Lorenz T. Biegler
Carnegie Mellon University
Pittsburgh, USA
biegler@cmu.edu

PP1
Regime-switching Competitive Lotka-Volterra Ecosystems Involving a Singularly Perturbed Markov Chain

We consider regime-switching competitive Lotka-Volterra models involving a singularly perturbed Markov chain. After examining the existence and uniqueness of solutions, we study crucial issues as permanence and extinction. Along this line, we also establish a number of properties such as moment boundedness, tightness, positive recurrence etc. The Markov chain in the singularly perturbed systems has a countable state space, which is fast varying. Under suitable conditions, we show that there are limit systems associate with the original model. We will demonstrate how to use the limit systems to study the behavior of the original systems. In addition, designing feedback controls to make the systems permanent or extinct will be considered as well.

Trang Bui
Wayne State University
trang.bui@wayne.edu

George Yin
Wayne State University
Department of Mathematics
gyin@math.wayne.edu

PP1
Performance of Distributed Lagrangian Methods for Network Resource Allocation with Uncertainty

Motivated by a variety of applications in control systems and computer networks, we consider distributed resource allocation problems, where the goal is to optimally allocate a limited number of resources to a group of nodes communicating over a dynamic network. In these problems, the scale of networks is often very large with complicated inter-connections between nodes, resulting in the need for distributed algorithms where the nodes are only allowed to interact with their local neighbors. We present here a novel distributed approach, namely, a distributed Lagrangian method, for resource allocation problems, while explicitly accounting for resource uncertainty. Unlike the well-known Lagrangian methods, our algorithm is attractive in that it circumvents the need for any form of central coordination to update the Lagrange multipliers. Our main contribution is to show that the distributed Lagrangian method is robust to the resource uncertainty while having good scalability with respect to the size of the network. Specifically, the algorithm has an asymptotic convergence in expectation to the optimal value with a rate $\mathcal{O}(n\ln(k)/(1-\sigma_2)\sqrt{k})$, where k is the number of iterations, n is the network size, and σ_2 represents the connectivity of the network. Finally, to illustrate the effectiveness of the proposed methods we apply them to study the important economic dispatch problems on the benchmark IEEE-14 bus systems.

Thinh T. Doan, Carolyn L. Beck
Coordinated Science Lab
University of Illinois at Urbana-Champaign
ttdoan2@illinois.edu, beck3@illinois.edu

PP1
Reduction of Linear Multivariable System Described by Internally Proper Polynomial Matrix Descriptions (PMDs) into an Equivalent State Space Model

A new algorithm is proposed for obtaining an equivalent state-space representation of a linear multivariable system whose dynamics are expressed by internally proper Polynomial Matrix Descriptions (PMDs) . These state-space formulations are used to analyze and examine certain properties of the associated PMD . It is shown that the concept of internal properness of a PMD , which is associated with the behavior and the output at time t = 0 , plays a crucial role in the transformation into a Fuhrmann equivalent model in state space form as is characterized by the absence from the matrices of poles/zeros at infinity . This requirement is important in linear systems theory in areas as composite system studies , system invertibility and minimality of system descriptions. Another consequence of the internal properness of the PMD is that it possesses no infinite input/output decoupling zeros and infinite system zeros. Hence the desired transformation has to preserve the basic properties of the PMD only in the finite frequencies.

George F. Fragulis
Western Macedonia Univercity of Applied Science
gfraguli@teiwm.gr

PP1
Applications of Multiple-scale Time Analysis and Different Pseudospectral Methods Along with MTM for CDF to Modeling, Estimation, Control, and Optimization of Large Scale Systems with Big Data

The challenges posed by the explosion in the availability of big data from different areas of study are changing the scope of many problems especially in systems dynamical, with different time scales, and of discontnuous nonlinear control. Besides well developed methods for multiple-scale analysis(of matched asymptotic expansions, WKB, combinations of different pseudospectral methods) this paper presents a new method based on different properties of Brownian motion, Cumulant Analysis, Theory of Associated Random Variables, and Time Series analysis for changes of Cumulative Distribution Function in relation to time change in sampling patterns. Multidimensional Time Model for Probability Cumulative Function can be reduced to finite-dimensional time model, which can be characterized by Boolean algebra for operations over events and their probabilities and index set for reduction of infinite dimensional time model to finite number of dimensions of time model considering also the fractal-dimensional time arising from alike supersymmetrical properties of probability. It is based on the properties of composition of Brownian

motion processes applied through application of Boolean prime ideal theorem and Stone duality. This model can be successfully applied in spatially ordered manner where the other mathematical models and simulations for Modeling, Estimation, Control, and Optimization of Large Scale Systems with Massive Data require complicated mathematical apparatus.

Michael Fundator
Sackler Colloquium, National Academy of Sciences of USA
michaelfundator@gmail.com

PP1
Local Poisson Equations Associated with Markov Control Model

This poster is concerned by a (discrete-time) controlled Markov processes $M = \langle S, A, C, P \rangle$ with denumerable state space S and a finite control space A. The performance of a policy π is measured by the long-run (superiorlimit) average cost at $x \in S$ which is defined by $J(\pi, x) := \limsup_n \frac{1}{n} J_n(\pi, x)$, where $J_n(\pi, x)$ is the total cost incurred before time $n > 0$ when the processes begin at estate x, $J_n(\pi, x)$ is defined by $J_n(\pi, x) := \lg(E_x^\pi [e^{\sum_{t=0}^{n-1} C(X_t, A_t)}])$. Let Π be the class of all policies for the model M, the optimal average cost function is determined by $J^*(x) := \inf_{\pi \in \Pi} J(\pi, x)$. In the present context, the following are the main results presented:
Result 1: If the one-step cost function C is nonnegative and has finite support, then the optimal average cost function can be obtained from a system of local Poisson equations which allows to obtain an optimal stationary policy.
(A system of Local Poisson equations is an object formally presented in this poster.) The second main result is
Result 2: If some finite subset F of the state space S is accessible from any initial state under any stationary policy, then there exists a system of local Poisson equations.
References:
Cavazos-Cadena, R., Hernández-Hernández, D.: Local Poisson equations associated with the Varadhan functional . Asymptotic Analysis. 96,(2015)

Diego L. Hernández
Centro de Investigación en Matemáticas, A. C.
CIMAT
diego.hernandez@cimat.mx

PP1
Splitting Collective Motion: Geometry of Kinematic Modes

We present a differential geometric framework for decomposition of the dynamics of n-particle systems into elementary motions, here referred to as *kinematic modes*. This framework can be applied in the analysis of collective motion (flocking) in nature and the synthesis of coordinated movements in robotic multi-agent systems. Snapshots of collective motion are modeled as tangent vectors on the configuration space of the n-particle system, with length given by the total kinetic energy. A fiber bundle structure and a connection in the sense of Ehresmann, are constructed to achieve splitting of a snapshot into modes tangential to lower-dimensional manifolds derived from configuration space. In this framework, we derive a decomposition of collective motion into first-order (rigid translations), second-order (inertia tensor transformations) and higher-order terms. This novel decomposition is interleaved with the classical decomposition of collective motion into rigid motion and shape transformation terms, yielding a rich family of kinematic modes. The allocation of kinetic energy among the different modes, and its evolution in time, can be used in the analysis of empirical data from natural collective phenomena, as illustrated on a published flocking dataset. In robotic multi-agent applications, collective motions that activate specific kinematic modes can be designed in the corresponding lower-dimensional manifolds, and conveniently combined in bottom-up fashion.

Matteo Mischiati
HHMI Janelia Research Campus
mischiatim@janelia.hhmi.org

P. S. Krishnaprasad
University of Maryland
krishna@isr.umd.edu

PP1
Data Assimilation and Electrophysiological Modeling of Mammalian Circadian Clock Neurons

Recently there has been interest in the application of data assimilation tools to the improvement of neuronal models. Often, the only data one has access to is the measured voltage from a current-clamp experiment with a prescribed injected current. Our work aims to improve understanding of the impact that injected current stimuli has on the identifiability of parameters in a neuronal model. Parameter estimation results will be shown from 4D-variational data assimilation (4D-var) and an Unscented Kalman Filter (UKF). We will test the performance of characteristic currents, including steps and ramps, as well as chaotic currents and currents optimized to uncover the full dynamic range of the gating variables. The ability of these various stimulus protocols to enable state and parameter estimation will be assessed using simulated data from the Morris-Lecar model and a biophysical model of mammalian circadian clock neurons in the suprachiasmatic nucleus.

Matthew Moye
Department of Mathematical Sciences
New Jersey Institute of Technology
mjm83@njit.edu

PP1
Control Performance of Connected and Automated Vehicles with Communication Erasure Channels

Connected and automated vehicles require integrated design of communications and control to achieve coordination of highway vehicles. Random features of wireless communications result in uncertainties in networked systems and impact control performance. Here we model switching network topologies by Markov chains and examine the impact of communication erasure channels on vehicle platoon formation and robustness under a weighted and constrained consensus framework. By comparing convergence properties of networked control algorithms under different communication channel features, we characterize some intrinsic relationships between packet delivery ratio and convergence rate. Simulation case studies are performed to verify the theoretical findings.

Thu T. Nguyen, Le Yi Wang
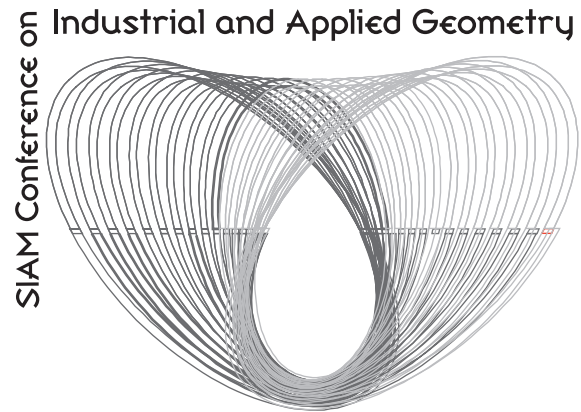Wayne State University
fw6622@wayne.edu, lywang@wayne.edu

George Yin

Wayne State University
Department of Mathematics
gyin@math.wayne.edu

Hongwei Zhang
Wayne State University
hongwei@wayne.edu

SP1

AWM-SIAM Sonia Kovalevsky Lecture: Mitigating Uncertainty in Inverse Wave Scattering

Inverse wave scattering is an inverse problem for the wave equation, driven by a broad spectrum of applications. It is an interdisciplinary area that involves mathematical analysis, computational modeling, statistics and signal processing. This lecture will discuss one important challenge due the uncertainty of the model for inversion. Uncertainty is unavoidable in applications, not only because of noise, but because of lack of detailed knowledge of complex media through which the waves propagate.

Liliana Borcea
University of Michigan
borcea@umich.edu

SP2

The John Von Neumann Lecture - Singular Perturbations in Noisy Dynamical Systems

Consider a deterministic dynamical system in a domain containing a stable equilibrium, e.g., a particle in a potential well. The particle, independent of initial conditions eventually reaches the bottom of the well. If however, a particle is subjected to white noise, due, e.g., to collisions with a population of smaller, lighter particles comprising the medium through which the Brownian particle travels, a dramatic difference in the behavior of the Brownian particle occurs. The particle can exit the well. The natural questions then are: how long will it take for it to exit and from where on the boundary of the domain of attraction of the equilibrium will it exit. We compute the mean first passage time to the boundary and the probability distribution of boundary points being exit points. When the noise is small each quantity satisfies a singularly perturbed deterministic boundary value problem. We treat the problem by the method of matched asymptotic expansions (MAE) and generalizations thereof. MAE has been used successfully to solve problems in many applications. However, there exist problems for which MAE does not suffice. Among these are problems exhibiting boundary layer resonance, which led some to conclude that this was "the failure of MAE". We present a physical argument and four mathematical arguments to modify MAE to make it successful. Finally, we discuss applications of the theory.

Bernard Matkowsky
Northwestern Universtiy, USA
b-matkowsky@northwestern.edu

SP3

Past President's Address: The Future of SIAM: Looking to the Mathematicians of Tomorrow

During my tenure as SIAM president, I sought to emphasize that the S in SIAM stands for students by focusing on boosting our global presence and cultivating the next generation of mathematicians. To all the long-time SIAM members, can you guess how many new international chapters weve added since 2012? To all the new SIAM student members weve welcomed in that period, can you name all the ways SIAM can help you grow your careers? At the 2017 SIAM Annual Meeting I will invite our Student Chapters to use their own words to answer these important questions through a series of videos spanning several continents. The advances weve made should make us all proud. Of course, theres always more that SIAM can do

as it continues to push ahead in order to remain at the vanguard of the scientific community.

Irene Fonseca
Carnegie Mellon University
Center for Nonlinear Analysis
fonseca@andrew.cmu.edu

SP4

James H. Wilkinson Numerical Analysis and Scientific Computing Prize Lecture: Tensors in Computational Mathematics

We show that in many instances, one would find a higher-order tensor, usually of order three, at the core of an important problem in computational mathematics. The resolution of the problem depends crucially on determining certain properties of its corresponding tensor. We will draw examples from (i) numerical linear algebra: fastest/stablest algorithms for matrix product, matrix inversion, or structured matrix computations; (ii) numerical optimization: SDP-relaxations of NP-hard problems, self-concordance, higher-order KKT conditions; and, if time permits, (iii) numerical PDEs: tensor network ranks. This talk is based on joint works with Ke Ye, with Shenglong Hu, and with Shmuel Friedland.

Lek-Heng Lim
University of Chicago
lekheng@galton.uchicago.edu

SP5

I.E. Block Community Lecture: From Flatland to Our Land: A Mathematicians Journey through Our Changing Planet

Mathematics is central to our understanding of the world around us. We live in a vast dynamical system, the many dimensions of which can be interrogated with mathematical tools. In this talk I will consider our changing climate. I will describe the scientific evidence that tells us how and why our climate is changing, and what the future may hold. In this journey I will pause at various waypoints to describe in more detail some of the insight different branches of mathematics are providing. Diverse examples will include applying ideas from dynamical systems research to create novel strategies for measuring the ocean mixing processes that are critical to the flow of heat and carbon through the Earth system, through to employing statistical learning techniques to improve future predictions of Arctic sea ice, currently in perilous decline. Climate change is one of the greatest challenges facing humanity. Responding to the challenge requires robust scientific evidence to inform policies. Opportunities for mathematicians to contribute to this important issue abound.

Emily Shuckburgh
British Antarctic Survey, United Kingdom
emily.shuckburgh@bas.ac.uk

JP1

AN17 and CT17 Joint Plenary Speaker - Bio-Inspired Dynamics for Multi-Agent Decision-Making

I will present a generalizable framework that uses the singularity theory approach to bifurcation problems, and other tools of nonlinear dynamics, to translate some of the remarkable features of collective animal behavior to an ab-

stract agent-based model. With the abstract model, analysis and design of decision-making between alternatives can be systematically pursued for natural or engineered multi-agent systems. To illustrate, I will apply the framework to explore and extend value-sensitive decision-making dynamics that explain the adaptive and robust behavior of house-hunting honeybees

Naomi E. Leonard
Princeton University
naomi@princeton.edu

CP1

Interpolation on Symmetric Riemannan Spaces.

Cubic spline interpolation on Euclidean space is a standard topic in numerical analysis, with countless applications in science and technology. In several emerging fields, for example computer vision and quantum control, there is a growing need for spline interpolation on curved, non-Euclidean space. The generalization of cubic splines to manifolds is not self-evident, with several distinct approaches. One possibility is to mimic the acceleration minimizing property, which leads to Riemannian cubics. They, however, require the solution of a coupled set of non-linear boundary value problems that cannot be integrated explicitly, even if formulae for geodesics are available. Another possibility is to mimic de Casteljau's algorithm, which leads to generalized Bezier curves. To construct C^2-splines from such curves is a complicated non-linear problem. Here we provide an iterative algorithm for C^2-splines on symmetric spaces, and we prove convergence under a verifiable set of conditions. In terms of numerical tractability and computational efficiency, the new method surpasses those based on Riemannian cubics. Each iteration is embarrassingly parallel, thus suitable for multi-core implementation. We demonstrate the algorithm for three geometries of interest: the n-sphere, complex projective space, and grassmannian manifolds. Joint work with Klas Modin, Chalmers, and Olivier Verdier, Bergen University College

Geir Bogfjellmo
Chalmers University of Technology
geir.bogfjellmo@chalmers.se

CP1

An Iterative Approach to Barycentric Rational Hermite Interpolation

In this paper we study an iterative approach to the Hermite interpolation problem, which first constructs an interpolant of the function values at $n+1$ nodes and then successively adds m correction terms to fit the data up to the m-th derivatives. In the case of polynomial interpolation, this simply reproduces the classical Hermite interpolant, but the approach is general enough to be used in other settings. In particular, we focus on the family of barycentric rational Floater–Hormann interpolants, which are based on blending local polynomial interpolants of degree d with rational blending functions. For this family, the proposed method results in rational Hermite interpolants with numerator and denominator of degree at most $(m+1)(n+1)-1$ and $(m+1)(n-d)$, respectively, which converge at the rate of $O(h^{(m+1)(d+1)})$ as the mesh size h converges to zero. After deriving the barycentric form of these interpolants, we prove the convergence rate for $m=1$ and $m=2$, and experimentally show that the approximation results compare favourably with other constructions.

Emiliano Cirillo, Kai Hormann
Università della Svizzera italiana
cirile@usi.ch, kai.hormann@usi.ch

CP1

From Big Data to Smart Data: Modelling Big Data Using Locally Refined Splines

Generating and analysing big datasets is not a new challenge in science and engineering. From seismic surveys of potential oil fields to meteorological models: the availability of storage space and computational resources have always been central limitations for the size and complexity of the problems we can solve. As processing power and storage space have become cheaper and more efficient, companies such as Google and Facebook have developed massively distributed infrastructures and algorithms to extract valuable information from enormous datasets. These Big Data tools have focused on data such as customer databases and personal status updates, which can easily be divided into manageable chunks. Such tools are now also used in the fields of science and engineering. However, the intrinsic structure of these data brings new challenges, and necessitates the adaption of existing Big Data methods and infrastructures. On the other hand, the spatial and physical structures in our data provide additional information which should be exploited when mining these datasets for information. In this presentation we will describe how Locally Refined (LR-) splines have been used to approximate Big 2D and 3D Data, creating interactive models well-suited for GPU visualization and analytics. Drawing on our experiences in two recently completed European Big Data projects, IQmulus and VELaSSCo, we describe some of the challenges of implementing these algorithms in Big Data infrastructures.

Heidi Elisabeth I. Dahl
SINTEF DIGITAL
heidi.dahl@sintef.no

Tor Dokken
SINTEF ICT, Department of Applied Mathematics
Oslo, Norway
tor.dokken@sintef.no

Oliver Barrowclough
SINTEF
Norway
oliver.barrowclough@sintef.no

CP1

Approxately Continuous Scatter Data Interpolation

In an approximately C^1 continuous surface, we have surface patches that meet with C^0 continuity where there is a bound on the angle between normals of two patches meeting along the C^0 join. In this talk, we give constraints on the control points for two bi-quadratic tensor product patches or two cubic triangular Bezier patches to meet approximately C^1 while meeting a specified angle constraint. We use these patches in a variation of Clough-Tocher to interpolate scattered data.

Stephen Mann
Cheriton School of Computer Science
University of Waterloo

smann@uwaterloo.ca

Xiang Fang
University of Waterloo
x2fang@uwaterloo.ca

CP2

Recovery of Geometrical, Topological and Transport Properties of Porous Rocks from Micro-Ct Images

We discuss the problem of determination of an optimal combination of resolution and image size of CT-scan for obtaining statistically reliable estimation of geometrical, topological and physical properties of a typical sandstone rock. The CT-scan 3D image can be considered as union two bodies: pore space P and matrix M. The geometrical properties of P can be described by their integral characteristics: volume, surface area, integral mean curvature and Euler characteristics. The computation of these characteristics can be achieved with help of the Minkowski functionals. The Euler characteristics represents topological properties of P, which more generally expressed by the Betti numbers b_0, b_1, b_2. To avoid dependence of Betti numbers on noise consisting of small components of P we use volume-weighted Betti numbers. In order to obtain more delicate estimates of the topological structure of P which can reflect its transport properties we suggest to use persistent homology of the filtration of P by sequence of decreasing bodies $P \supset P_1 \supset \ldots$ obtained by dilation of matrix M. Corresponding persistence diagram expresses multiscale nature of pore space and reflects the structure of pores and thresholds with different sizes. There are some evidences that the diagram correlates to transport properties of sample.

Yaroslav Bazaikin
Inst. of Mathematics of SB RAS
Russia
bazaikin@gmail.com

Boris Gurevich
Curtin University
b.gurevich@curtin.edu.au

Tatyana Khachkova
Inst. of Petroleum Geology and Geophysics SB RAS
Russia
khachkovats@ipgg.sbras.ru

Dmitriy Kolyukhin
(a) Trofimuk Institute of Petroleum Geology and Geophysics
SB RAS Novosibirsk, Russia; (b) Uni CIRP, Bergen, Norway
KolyukhinDR@ipgg.sbras.ru

Maxim Lebedev
Curtin University
m.lebedev@exchange.curtin.edu.au

Vadim Lisitsa
Institute of Petropeum Geology & Geophysics of SB RAS
Russia
lisitsavv@ipgg.sbras.ru

Vladimir Tcheverda
Inst. of Petroleum Geology and Geophysics SB RAS

Russia
cheverdava@ipgg.sbras.ru

CP2

Applications of Multidimensional Time Model for Probability Cumulative Function to Geometrical Predictions

Multidimensional Time Model for Probability Cumulative Function can be reduced to finite-dimensional time model, which can be characterized by Boolean algebra for operations over events and their probabilities and index set for reduction of infinite dimensional time model to finite number of dimensions of time model through application of Boolean prime ideal theorem and Stone duality and can be indexed by an index set considering also the fractal-dimensional time arising from alike supersymmetrical properties of probability through consideration of extension of the classical Stone duality to the category of Boolean spaces, locally compact Hausdorff spaces. The introduction of probabilistical prediction philosophically based on Erdos- Reney Law for the prediction through Descartes cycles, Gauss methods of trigonometric interpolation and least squares to reduce error in determination of the orbits of planetary bodies, and Farey series continued by sampling on the Sierpinski gasket.

Michael Fundator
Sackler Colloquium, National Academy of Sciences of USA
michaelfundator@gmail.com

CP2

A New Model for the Biofilm Growth Evolution in a Porous Medium and Its Effects in the Characteristics of the Porous Medium

Microbial enhanced oil recovery (MEOR) aims at microbial growth to increase oil production. Different grades of success have been observed in MEOR techniques. For this reason, the existence and use of more precise models of the recovery of oil by means of bacterial growth are crucially important for determining the feasibility of this technique [Sen, "Biotechnology in petroleum recovery: the microbial eor, 2008]. In this work, we model the growth of bacteria on a microscopic scale in a porous medium. We used a network model to describe flow through a porous medium and we used a new formalism for the growth of bacteria that describes the distribution of the bacteria through the entire network. We studied the changes in porosity and permeability caused by bacteria growth and we found a phenomenological analytical relation between the permeability and a number of bacteria in the network. We intend to use this phenomenological relation for the up-scaling of this model to the continuum scale.

Luis A. Lopez
Institute of Applied Mathematics, TU Delft
luisantoniolopezp@gmail.com

CP2

Selecting Minimum Explaining Variables by Pruned Primary Ideal Decomposition with Recursive Calls

Jarrah et al. (2007) proposed an algorithm using the primary decomposition of monomial ideals for selecting minimum wiring diagrams for biological gene networks (or

input-output relationships with polynomial functions in general) from finite observations of a set of variables. However, its computational cost with computer algebra system is relatively high, preventing the practical applications to the big data. Here we implemented the algorithm in the form of recursive calls in Matlab and approximated it by pruning the search trees to consider only the cases with the minimum number of explaining variables. This speed-up enabled us to treat larger data of about 100x100 size.

Keiji Miura
Kwansei Gakuin University
miura@kwansei.ac.jp

CP2
Metamaterial Lens Design

We prove how to design a lens that focuses monochromatic radiation from a light source into a given point when the lens is constructed out of an exotic material known as a Metamaterial (meta = $\mu\varepsilon\tau\alpha$ = "beyond" in Greek). Such materials do not exist naturally, but have been constructed in the laboratory in the early 2000's. The research on the behavior of these materials has been extremely active in recent years, especially for applications to invisibility cloaking and the development of a "superlens", which can in principle image objects at the smallest scales. In this talk I will discuss the precise construction of the lens; i.e., given one surface of the lens, we construct the second surface explicitly, and show that most of the time the slab has a non-rectangular geometry, even if the given surface is planar. This is joint work with Cristian Gutiérrez.

Eric Stachura
Temple University
estachura@haverford.edu

Cristian Gutierrez
Department of Mathematics
Temple University
gutierre@temple.edu

CP3
Folding Flat Plates Using Surface Tension

Alternative to standard methods of micro-scale fabrication that rely on the stacking patterned thin films, surface-tension-driven folding, or capillary origami, has been proposed as a feasible approach for turning planar objects into three-dimensional structures. Its utility is at small scales interfacial forces dominate over bulk forces so that resulting configurations are energetically preferred and, in turn, passively achieved. A main challenge in determining the possible 3D shapes formed by capillary origami is predicting the behavior of large, nonlinear elastic deformations of a thin plate. Mathematically, this can be stated as finding isometrically constrained minimizers of a Willmore-type functional. This talk will focus on constructing such minimal bendings in a simple situation and discuss the challenges of generalizing such a procedure.

Nicholas D. Brubaker
University of Arizona
nbrubaker@fullerton.edu

CP3
Adaptive Grids for Accurate Visualizations of

Complex Function Data

The NIST Digital Library of Mathematical Functions (DLMF) (http://dlmf.nist.gov/) contains close to 600 graphical representations of complex mathematical functions. More than 200 of these are interactive 3D surface visualizations that have evolved with the emergence of technology for rendering 3D graphics on the web. While the quality of most of the visualizations is quite good, in some cases color maps and areas around key features such as poles, zeros and branch cuts could be enhanced by improving the underlying grid. The original grids, designed using simple structured techniques like transfinite blending function interpolation or variational methods and tensor product B-splines, could be generated separately from the function data. However, ideally we want to generate grids that adapt to curvature and gradient information gleaned from the function data, but this introduces the additional problem of linking the grid generation code to software used to compute the function data. This can be especially challenging when the most reliable software for computing values of a particular mathematical function is only available in a specific language or package. We discuss our success to date and make some suggestions for future work.

Bonita V. Saunders
National Institute of Standards and Technology (NIST)
bonita.saunders@nist.gov

CP3
Parametric Finite Elements with Bijective Mappings

The discretization of the computational domain plays a central role in the finite element method. In the standard discretization the domain is triangulated with a mesh and its boundary is approximated by a polygon. The boundary approximation induces a geometry- related error which influences the accuracy of the solution. To control this geometry-related error, iso-parametric finite elements and iso-geometric analysis allow for high order approximation of smooth boundary features. We present an alternative approach which combines parametric finite elements with smooth bijective mappings leaving the choice of approximation spaces free. Our approach allows to represent arbitrarily complex geometries on coarse meshes with curved edges, regardless of the domain boundary complexity. The main idea is to use a bijective mapping for automatically warping the volume of a simple parameterization domain to the complex computational domain, thus creating a curved mesh of the latter. The numerical examples confirm that our method has lower approximation error than the standard finite element method, because we are able to solve the problem directly on the exact shape of domain without having to approximate it.

Patrick Zulian
Università della Svizzera italiana, Switzerland
patrick.zulian@usi.ch

Teseo Schneider
Universita della Svizzera Italiana
teseo.schneider@usi.ch

Kai Hormann
Università della Svizzera italiana
kai.hormann@usi.ch

Rolf Krause

Università della Svizzera italiana, Switzerland
rolf.krause@usi.ch

CP3
Optimization in Shape Spaces

Shape optimization problems arise frequently in technological processes which are modelled by partial differential equations (PDEs). In many practical circumstances, the shape under investigation is parametrized by finitely many parameters. This allows the application of standard optimization approaches, but limits the space of reachable shapes unnecessarily. Shape calculus presents a way to circumvent this dilemma. However, so far it is mainly applied in the form of gradient descent methods, which can be shown to converge. The major difference between shape optimization and the standard PDE constrained optimization framework is the lack of a linear space structure on shape spaces. We consider optimization problems which are constrained by PDEs and embed these problems in the framework of optimization in shape spaces. A lot of techniques for PDE constrained shape optimization problems are based on the so-called Hadamard-form of shape derivatives, i.e., in the form of integrals over the surface of the shape under investigation. It is often a very tedious process to derive such surface expressions. Along the way, there appear volume formulations as an intermediate step. Volume integral formulations of shape derivatives are coupled with optimization strategies on shape spaces. Efficient shape algorithms reducing analytical effort and programming work are presented and a novel shape space is proposed in this context.

Kathrin Welker
Trier University
welker@uni-trier.de

Volker H. Schulz
University of Trier
Department of Mathematics
Volker.Schulz@uni-trier.de

Martin Siebenborn
Department of Mathematics
University of Trier
siebenborn@uni-trier.de

CP3
Mesh Denoising Based on Normal Voting Tensor and Binary Optimization

Mesh denoising is a central preprocessing tool in discrete geometry processing with many applications in computer graphics such as CAD, reverse engineering, virtual reality and medical diagnosis. The acquisition of 3D surface data takes place using 3D measurement technologies such as 3D cameras and laser scanners. During the surface measurement, noise is inevitable due to various internal and external factors. This degrades surface data quality and its usability. The main goal of any mesh denoising algorithm is to remove spurious noise and compute a high quality smooth function on the triangle mesh while preserving sharp features. We would like to present a novel tensor multiplication based mesh denoising algorithm. Unlike other traditional averaging approaches, our approach uses an element based normal voting tensor to compute smooth surfaces. By introducing a binary optimization on the proposed tensor together with a local binary neighborhood concept, our algorithm better retains sharp features

and produces smoother umbilical regions than previous approaches. On top of that, we provide a stochastic analysis on the different kinds of noise based on the average edge length. The quantitative results demonstrate that performance of our method is better compared to state of the art smoothing approaches.

Sunil K. Yadav, Ulrich Reitebuch
Free University Berlin
sunil.yadav@fu-berlin.de, ulrich.reitebuch@fu-berlin.de

Konrad Polthier
Freie Universitaet Berlin
FB Mathematik & Informatik
konrad.polthier@fu-berlin.de

MS1
A Life of Quality Affecting Many People

Abstract Not Available At Time Of Publication.

Robert Barnhill
Vice President for Science Policy & Strategic Initiatives,
Society for the Advancement of Chicanos and Native
Americans
robert.barnhill@asu.edu

MS1
Geralds Life and Work - the Early Years

Abstract Not Available At Time Of Publication.

Hans Hagen
Department of Computer Science
University of Kaiserslautern
hagen@informatik.uni-kl.de

MS1
Making Gk Simple - Spline Manifolds by Farins Ck Construction

In his 1979 thesis, Gerald Farin carried Staerk's simple Ck condition for curves over to triangular Bzier representations. It took about 10 years untill the CAGD community realized that more general Gk conditions are necessary to build arbitrary smooth freeform surfaces. For surfaces however, Gk conditions lack the very useful simple geometric representation of Farin's Ck condition. Still Gerald was convinced that it should be possible to construct arbitrary smooth surfaces by simple or at least geometric constructions. And in fact he has been right after all: Homogenous splines representing arbitrary rational Gk spline manifolds satisfy Gerald's Ck conditions for tetrahedral Bzier representations. Moreover, their rational Bzier representations satisfy the projective version of his Ck condition where weight points come into play, another invention of Gerald. In this talk I will explain these and further basics and show how they can be applied to build everywhere smooth rational and integral Gk splines consisting either of triangular or quadrilateral tensor product patches with a polycube structure.

Hartmut Prautzsch
Universitaet Karslruhe

prautzsch@kit.edu

MS2

Topological Properties of Meandering Streams

Modeling a meandering stream in geological settings should include layering effects based on sedimentary processes. It is assumed that different layers in the model were created by ocean bearing material settling to the ocean bottom. The topological modeling of a water-created stream bed relies on a volumetric representation with a point membership function, a surface function to support ray theory methods, and an internal method of parameter representation of physical properties. Methods in use include finite elements and Bezier surfaces in 2D and 3D. The role of isoparametric finite element methods (Schemes of Bruce Irons) will be shown, with discussion of the topological issues, focusing upon the continuity of functions and derivatives, as step changes in material properties occur at boundaries. These models are of interest for industrial exploration of the complex geological subsurface.

Ralph P. Bording
Alabama A&M University
philbording@hotmail.com

MS2

Hierarchical Metric Trees for Topological Data Analysis

Hierarchical trees represent a metric space at different scales and each level of the tree samples the data at a different scale. Understanding multiscale geometric structure is an important problem in topological data analysis, a field that seeks to efficiently reveal the underlying shape of data. Here, we show that how such trees can be used to extract some meaningful features of a data set.

Mahmoodreza Jahanseirroodsari
University of Connecticut
mahmoodreza.jahanseirroodsari@uconn.edu

MS2

Topology in Artistic Expression

For artistic expression, existing motion capture data gloves were seen as cumbersome, while also limited by not being deployed over both hands. Inexpensive solutions will be presented through topological extensions to interactive graphics algorithms to provide haptic feedback for manipulation of geometric objects.

Kevin Marinelli
University of Connecticut
Computer Science and Engineering
kevin.marinelli@uconn.edu

MS2

Knot Theory and Computational Steering for Molecular Simulations

The knot equivalence of isotopy is a useful mathematical model for computational steering algorithms to examine temporal changes in molecular configurations. The molecules have been modeled as Bezier curves, leading to new approximation methods that have implications for studying theoretical issues for stick knots.

Thomas J. Peters
University of Connecticut
tjp5k82@gmail.com

MS3

Geometric Modeling and Processing in Irit

Abstract Not Available At Time Of Publication.

Gershon Elber
Technion, Haifa
Israel
gershon@cs.technion.ac.il

MS3

Predictive Shimming Through Scripted Process Engineering

Abstract Not Available At Time Of Publication.

Dan Gonsor
The Boeing Company
daniel.e.gonsor@boeing.com

MS3

Scripted Process Engineering at Boeing

Abstract Not Available At Time Of Publication.

Thomas A. Grandine
Applied Mathematics
The Boeing Company
thomas.a.grandine@boeing.com

MS3

Adaptive Geometric Modeling

Industrial products are usually designed through (commercial) Computer Aided Design (CAD) systems based on the B-spline technology and its non-uniform rational extension (NURBS). To overcome the limitations of their tensor-product structure, the recently developed truncated hierarchical B-splines (THB-splines) have been integrated into the geometric modeling environment of MTU Aero Engines AG.

The Minisymposium talk will introduce the use of THB-splines for the (re)-design of aircraft engine components, for example within the surface fitting part of the process for reconstructing CAD models from (optical) measured data. Furthermore, we will demonstrate how to combine THB-splines with commercial geometric modeling kernels and their exact conversion into CAD geometry. As a consequence, the adaptive modeling tool can be fully integrated into CAD systems that comply with the current NURBS standard and provide modeling operations like blending, thickening and trimming.

David Gromann
MTU Aero Engines, Germany
david.grossmann@mtu.de

MS4

Analytic Methods for Modern Design and Manu-

facturing

Abstract: Mathematical morphology provides a strong foundation for creation of computational design tools for additive/subtractive manufacturing, including manufacturability analysis, planning, and design correction for solid parts made by depositing or removal of materials. This talk overviews some of the recent developments, existing challenges, and future directions in applying such tools to digital design and manufacturing. In particular, I will discuss an emerging paradigm of 'analytic methods' that reformulate a vast array of important geometric operations in the language of measure-theory, convolution algebra, and digital signal processing, and show its great promise for extending the computational design technology for traditional manufacturing to modern material structures and fabrication processes.

Morad Behandish
International Computer Science IInstitute
morad@icsi.berkeley.edu

MS4

A Circle Packing Heuristic with Applications to 3D Printing

Abstract Not Available At Time Of Publication.

John Bowers
James Madison University
bowersjc@jmu.edu

MS4

3D-Epug-Overlay: Intersecting Very Large 3D Triangulations in Parallel

We present 3D-EPUG-Overlay, an algorithm and preliminary implementation for intersecting (aka overlaying) two 3D triangulations. This operation is important in processing large geometry datasets in additive manufacturing. Much of our algorithm is a sequence of map-reduce operations, and so is easily parallelizable. We completely avoid roundoff errors and the associated topological problems by computing with rational numbers. We will handle geometric degeneracies with Simulation of Simplicity (SoS). Our target architecture is an inexpensive workstation. We have a complete 2D implementation, which has overlaid two 2D maps maps, with a total of 54,000,000 vertices and 739,000 faces, in only 322 elapsed seconds (excluding I/O) on a dual 8-core 3.4GHz Intel Xeon workstation. That time is using 16 cores, and is 11x faster than using one core. Our 3D implementation is complete except for SoS. It processes two 3D objects with a total of 6,000,000 face triangles and 3,000,000 tetrahedra in 180 elapsed seconds on 16 cores. The parallel speedup for 16 cores is a factor of 13. The execution time is almost linear in the data size, and could process much larger datasets, perhaps billions of triangles. We anticipate being able to process much larger datasets than competing SW can, and for datasets small enough for others to process, that we will be much faster and more robust on special cases.

Randolph Franklin
Rensselaer Polytechnic Institute
mail@wrfranklin.org

Salles Viana Gomes de Magalhães
Rensselaer Polytechnic Institute
Federal U of Viçosa, Brazil

sallesviana@gmail.com

MS4

Math by Design: 3D Printing for the Working Mathematician

Mathematicians often spend their days thinking about ideas that exist only in their minds. In this talk we'll discuss how to use 3D printing to bring models of those ideas into reality, from start to finish. We'll show how to leverage design software to convert mathematical objects into triangular meshes or voxel representations, and then how those digital representations become code that a 3D printer can understand and implement to create real-world objects. Learn how to get started creating your own mathematical 3D design files, level up your existing design skills, or just enjoy watching the process of turning abstract mathematics into physical plastic.

Laura Taalman
James Madison University
laurataalman@gmail.com

MS5

Particle Swarm Optimization for High-dimensional Stochastic Problems

Abstract Not Available At Time Of Publication.

Hongmei Chi
Department of Computer Science
Florida A&M University
hchi@cis.famu.edu

MS5

Optimizing Tree Width for Performance in the Walk-on-Spheres Algorithm

Abstract Not Available At Time Of Publication.

Derek Juba
NIST
derek.juba@nist.gov

MS5

Tree-Based Geometrical Decomposition and the Walk-on-Spheres Monte Carlo Algorithm

Abstract Not Available At Time Of Publication.

Walid Keyrouz
National Institute of Standards and Technology
Software and Systems Division
walid.keyrouz@nist.gov

MS5

Geometry Entrapment in Walk-on-Subdomains

Abstract Not Available At Time Of Publication.

Michael Mascagni
Computer Science/Computational Science
Florida State University, Tallahassee

mascagni@.fsu.edu

MS6
Rational Geometric Splines for Surfaces of Arbitrary Topology

Rational Geometric Splines (or RAGS) are piecewise functions that can be used to represent smooth parametric surfaces of arbitrary topological genus and arbitrary order of continuity. The main advantage of RAGS surfaces in comparison to alternative representations, for example those based on so-called manifold splines, subdivision methods and T-splines, is that they mimic the standard bivariate splines on planar domains and their constructive aspects, thus they are closer in spirit to the traditional NURBS representation. After reviewing the basics of RAGS, we will discuss how to construct these splines by suitable association with a homogeneous geometry. We will provide computational examples considering direct analogs of the Powell-Sabin macro-elements and also spline surfaces of higher degrees and higher orders of continuity obtained by minimizing an energy functional.

Carolina Beccari
Department of Mathematics, University of Bologna
carolina.beccari2@unibo.it

Mike Neamtu
Vanderbilt University
Department of Mathematics
neamtu@math.vanderbilt.edu

MS6
Adaptive Surface Reconstruction From Scattered Data by Hierarchical Splines

Surface reconstruction from scattered data is a relevant problem in a wide range of applications, which has been approached with a variety of solutions. The irregular configuration of the data naturally leads to adaptive methods which provide suitable local approximations according to the distribution and density of the data. We present a new scheme which approximates the data by a suitable quasi-interpolant (QI) in a hierarchical spline space (see, e.g., [C. Giannelli, B. Jüttler, and H. Speleers, THB-splines: The truncated basis for hierarchical splines. Comput. Aided Geom. Design, 29, 485- 498, 2012]). The QI, which is hierarchical in the sense of [H. Speleers and C. Manni. Effortless quasi-interpolation in hierarchical spaces. Numer. Math., 132, 155-184, 2016], is based on local least squares polynomial approximations, whose degree is adaptively chosen according to the data configuration (similarly to [O. Davydov and F. Zeilfelder. Scattered data fitting by direct extension of local polynomials to bivariate splines. Adv. Comp. Math., 21, 223-271, 2004]). An automatic procedure, based on the current error with respect to the data, the number of data points locally available and the smallest singular value of the local collocation matrices, iteratively selects the suitable hierarchical space and degrees of the local approximations. The possibility to use different local approximants within the same scheme is discussed as well.

Cesare Bracco
University of Florence
cesare.bracco@unifi.it

Carlotta Giannelli
Istituto Nazionale di Alta Matematica

Italy
carlotta.giannelli@unifi.it

Alessandra Sestini
University of Florence
alessandra.sestini@unifi.it

MS6
Spline Orbifold Constructions

Any closed surface of genus g can be cut open into a $4g$-gon and the hyperbolic plane can be tesselated by hyperbolic shifts of $4g$-gons. This implies that G^k smooth genus g spline surfaces can be parametrized over some hyperbolic $4g$-gon, where the hyperbolic shifts correspond to the rational linear transition maps defining its G^k joints. Such splines have been called orbifold splines by Wallner and Pottmann. In this talk, I will express G^k joints for rational polynomials with rational linear transition maps as simple C^k joints for their homogeneous integral representations and show how these can be used to construct piecewise rational G^k surfaces from prototype Bzier nets that only need to satisfy C^0 conditions along common boundaries and G^1-conditions at common vertices. Furthermore, I bridge the gap to Jorg Peters construction of integral G^1 splines with rational linear transition maps, present differences between constructions with triangular and quadrilateral patches, and discuss limitations and solutions for integral G^k splines consisting of quadrilateral patches.

Hartmut Prautzsch
Universitaet Karslruhe
prautzsch@kit.edu

MS6
Geometric Construction of Matrix Weighted Rational B-spline Surfaces with Arbitrary Topology

Rational curves and surfaces are widely used in CAGD, but the construction of rational curves and surfaces with real weights is not as easy as that for non-rational curves and surfaces. In this talk we present a generalization of real weighted rational curves and surfaces to matrix weighted rational curves and surfaces. In particular, B-spline or NURBS surfaces with arbitrary topology have been generalized to matrix weighted rational subdivision surfaces of which the shapes are controlled by control points and normal vectors specified at the control points. We show three potential applications of the proposed surface model. 1. Modeling high quality/fair surfaces or surfaces with salient features using control points and control normals; 2. Direct reconstruction of NURBS surfaces or subdivision surfaces from sampled data without solving large systems; 3. Construction of curvature continuous surfaces with arbitrary topology by matrix weighted rational subdivision with adaptively choosing control points and control normals.

Xunnian Yang
School of Mathematical Sciences, Zhejiang University,
China
Hangzhou 310027, China
yxn@zju.edu.cn

MS7
Capping Non-Uniform Extraordinary Points

Extraordinary points are necessary to construct arbitrary

topological spline surfaces which play a central role in isogeometric analysis. However, if the knot intervals are different for the edges connecting an extraordinary point, the blending functions for extraordinary points of the existing methods can have two local maxima. This talk will review the different methods to handle this problem in these years and also provide our new development on this problem whose blending functions have a single local maximum.

Xin Li
University of Science and Technology of China,
School of Mathematical Sciences, Hefei, China
lixustc@ustc.edu.cn

MS7
Refinable Surfaces with Irregular Layout

Subdivision surfaces naturally provide a nested sequence of refined representations. But their infinite recursion and possibly poor shape complicates their inclusion into industrial design infrastructure and post-processing, such as computing integrals near the extraordinary limit points. Geometrically smooth constructions for filling multi-sided holes, while compatible with existing infrastructure and meeting shape requirements, seem to lack refinability of their natural B-spline-like control net. This talk will discuss recent results (i) that improve the shape and formal smoothness of subdivision surfaces; (ii) highlight options and trade-offs for refinability of functions on G-spline surfaces; and (iii) explore singular parameterizations, both for the physical domain and for the deformation functions. Each of these constructions yields isogeometric spaces over unstructured meshes according to Groisser,Peters 2015.

Jorg Peters
University of Florida
jorg@cise.ufl.edu

Kestutis Karciauskas
Faculty of Mathematics and Informatics
Vilnius University
kestutis.karciauskas@maf.vu.lt

MS7
U-splines: Splines Over Unstructured Meshes

Isogeometric design and analysis is a growing area of research in computational engineering. In an isogeometric approach, the exact CAD representation is adopted as the basis for analysis. To unlock the full potential of isogeometric analysis depends strongly upon the analysis-suitable nature of the underlying geometry. Analysis-suitable geometry possesses a basis that is rich enough for both shape and solution representation. The exact analysis-suitable representation of smooth geometry is essential for correct solution behavior across many application domains. In this talk we will present U-splines. U-splines are a new analysis-suitable spline description which alleviates the challenges associated with building analysis-suitable smooth bases over unstructured grids. U-spline basis functions are positive, form a partition of unity, and are locally linearly independent and overcome the analysis-suitability mesh constraints required by T-splines (including near extraordinary points and T-junctions). We will also discuss the application of U-splines as a basis for isogeometric analysis.

Michael Scott

Civil and Environmental Engineering
Brigham Young University
michael.scott@byu.edu

Derek C. Thomas
Brigham Young University
Dept. of Physics and Astronomy
dthomas@byu.edu

Kevin B. Tew
Brigham Young University
tew@byu.edu

Michael Borden
NC State
mjborden@ncsu.edu

Zhihui Zou
Brigham Young University
n/a

MS8
Smooth Parameterization of Complex Domains with Bezier Triangles

In this talk, I will present our recent work on smooth parameterization of complex domains with Bezier triangles. Our approach is based on macro-element techniques such as Powell-Sabin split and Clough-Tocher split, where the dimension of the spline space over triangulations can be determined by their connectivity. For a complex domain with non-uniform rational B-spline represented boundary, we first create a polygonalization of the domain and then triangulate it. Over this triangulation, we use macro-element techniques to obtain basis of higher-order continuity over the domain. The boundary polygons are then replaced with curved rational Bezier triangles to obtain the exact geometry. I will show both 2D and 3D numerical examples and their applications in isogeometric analysis.

Xiaoping Qian, Songtao Xia
University of Wisconsin-Madison
qian@engr.wisc.edu, xia@engr.wisc.edu

MS8
Smooth Trajectory Planning with Obstacle Avoidance Based on Pythagorean-hodograph Spline Curves with Tension

Trajectory planning is a fundamental task in several fields which can be addressed in two successive phases, the first aimed to the identification of the path geometry and the second to the definition of a suited feedrate profile. Considering this setting in the planar case, when the path has to be designed within an environment with obstacles, we first identify a suitable admissible piecewise linear path which is then modified into a smooth path by using the G^2 interpolation scheme with tension based on PH curves introduced in the literature. The method is fully automatic since a new technique for the tension parameters selection is proposed in order to preserve the path collision avoidance. For the second phase we present a strategy for defining a C^2 time-dependent feedrate profile minimizing the traversal time and constrained by chord tolerance as well as by velocity, acceleration and jerk limitations. Since the PH structure of our paths ensure exact arc length computation, at real time an accurate and fast interpolator can be used to determine the sequence of positions along the path

associated with uniform time spacing, as required by any motion driver.

Alessandra Sestini
University of Florence
alessandra.sestini@unifi.it

Carlotta Giannelli
Istituto Nazionale di Alta Matematica
Italy
carlotta.giannelli@unifi.it

Duccio Mugnaini
University of Insubria
dmugnaini@uninsubria.it

MS8

Smooth Polar Splines for Isogeometric Analysis

One of the needs of CAD representations of arbitrary genus surfaces with finite number of polynomial patches is the introduction of holes surrounded by periodic configurations. Such holes can then be filled by means of polar spline surfaces, where the basic idea is to use periodic spline patches with one collapsed boundary. Applications of this approach include subdivision surfaces, free-shape modeling, and, as we demonstrate here, isogeometric analysis. In order to obtain polar spline surfaces with specified continuity, the admissible set of control point configurations shrinks. In particular, at the collapsed boundary (invoking a singular point), imposition of C^k continuity constrains the inner k-rings of control points surrounding the singular point to a limited number of configurations. In hole-filling applications, the outer k-rings of control points are used to match the cross-derivative information at the hole boundary. In this talk, keeping in mind applications to design as well as analysis, we focus on C^k polar spline parametric patches with arbitrary degree and arbitrary number of elements at the hole boundary. We present a simple, geometric construction of basis functions over such polar parametric domains possessing interesting properties as non-negativity and partition of unity. In addition, the constructed spline spaces show optimal approximation behavior, even at the singular point.

Hendrik Speleers
University of Rome "Tor Vergata"
speleers@mat.uniroma2.it

Deepesh Toshniwal
UT Austin
deepesh@ices.utexas.edu

Rene Hiemstra, Thomas J. R. Hughes
ICES
University of Texas at Austin
rene@ices.utexas.edu, hughes@ices.utexas.edu

MS8

General Framework for Approximation of Circular Arcs by G^k Parametric Polynomial Interpolants

Approximation of circular arcs by parametric polynomial curves is one of fundamental and well understood problems in computer aided geometric design. Since it is well known that circular arcs do not posses an exact polynomial representation, several approximation techniques have been proposed. The main goal is good approximation with re-spect to some prescribed error measure. Ideally, Hausdorff distance should be considered, but it is computationally expensive and difficult to analyze. Thus some alternative measures of distance have been introduced. Among all, radial distance turns out to be the most appropriate one, since under some additional constraints it coincides with Hausdorff measure. Approximants should usually fulfil some additional requirements, such as interpolation of end points of circular arc, interpolation its boundary tangent directions,... Such interpolants are commonly addressed as G^k interpolants. In this talk a general framework for optimal aproximation by G^k interpolants will be presented.

Ales Vavpetic
University of Ljubljana, Slovenia
ales.vavpetic@fmf.uni-lj.si

Emil Zagar
University of Ljubljana
Ljubljana, Slovenia
emil.zagar@fmf.uni-lj.si

MS9

Discrete (Multi-) Vector Field Design: Representations, Applications and Challenges

Direction fields and vector fields play an increasingly important role in applied geometry processing, with many applications in visual computing, computer graphics and simulation. To facilitate this wide range of applications, many different types of directional fields have been defined in the literature: from vector and tensor fields, over line and cross fields, to frame and vector-set fields. In addition to the type of vector field, researchers have also experimented with a large variety of application-specific objectives and constraints in order to synthesize such fields. Common notions of objectives include fairness, feature alignment, symmetry, specific field topology, among others. To facilitate these objectives, various representations, discretizations, and optimization strategies have been developed, each of which comes with varying strengths and weaknesses. This talk will present some of the notions, design choices, and challenges involved in designing discrete vector fields. We will look at some of the representations most commonly used in applications, with a slight focus on multi-vector fields, where more than one vectors or directions are assigned per point. We will highlight and compare two popular methods for design (implicit vs. explicit topology) and compare benefits and drawbacks. We will also look at various applications, such as mesh generation, deformation, texture mapping, and more.

Olga Diamanti
Stanford Univ.
diamanti@stanford.edu

MS9

Functional Approach to Vector Fields and Cross Fields

Tangent vector fields and cross fields appear in many areas of discrete geometry processing from texture design and analysis to physical simulation on curved surfaces. In this talk, I will describe a set of representations of tangent vector fields and cross fields based on considering their action on real-valued functions defined on the shapes. These representations facilitate global analysis and design of vector fields and cross fields, and allow to relate them to opera-

tions such as transfer across different shapes and the computation of vector field flow. I will give an overview of the properties of this functional representation and show some applications, including vector field design, fluid simulation, the computation of parallel transport, and consistent quadrangulation of pairs of shapes.

Maks Ovsjanikov
Ecole Polytechnique
maks@lix.polytechnique.fr

MS9
Boundary-Sensitive Hodge Decompositions

We provide a theoretical framework for discrete Hodge-type decomposition theorems of piecewise constant vector fields on simplicial surfaces with boundary that is structurally consistent with decomposition results for differential forms on smooth manifolds with boundary. In particular, we obtain a discrete Hodge-Morrey-Friedrichs decomposition with subspaces of discrete harmonic Neumann and Dirichlet fields, which are representatives of absolute and relative cohomology. Exciting open questions are related to the so-called Poincaré angle which appears as a feature of the decomposition on surfaces with positive genus. As applications, we compute refined Hodge-type decompositions of vector fields on surfaces with precise control along the boundary. The decompositions are well suited for vector field analysis, surface parametrization, remeshing and other geometry processing algorithms.

Konrad Polthier
Freie Universitaet Berlin
FB Mathematik & Informatik
konrad.polthier@fu-berlin.de

MS9
Vector Field Visualization with Gradient Tensor Analysis

Vector field visualization has contributed much to the understanding of vector fields in many scientific and engineering domains. On the other hand, much information about vector fields are embedded in their spatial gradients, i.e., the gradient tensor fields. In this talk, we review some recent advances in applying tensor field analysis to vector field visualization.

Eugene Zhang
Oregon State University
zhange@eecs.oregonstate.edu

MS10
Path Plannning with Generalized Barycentric Coordinates

Distance functions between points in a domain are sometimes used to automatically plan a gradient-descent path towards a given target point in the domain, avoiding obstacles that may be present. A key requirement for such distance functions is the absence of spurious local minima, which may foil such an approach, and this has led to the common use of harmonic potential functions. Based on the Laplace operator, the potential function guarantees the absence of spurious minima, but is well known to be slow to compute and prone to numerical precision issues. To alleviate the first of these problems, we propose a family of novel distances, based on f-divergence of the Poisson kernel. Our

first result is theoretical: We show that the family of divergence distances are equivalent to the harmonic potential function on simply-connected domains, namely they generate identical paths to those generated by the potential function. Our other results are more practical and relate to two special cases of divergence distances, one based on the Kullback-Leibler divergence and one based on the total variation divergence. We show that using divergence distances instead of the potential function and other distances has a significant computational advantage, as, following a pre-processing stage, they may be computed up to an order of magnitude faster. Furthermore, the computation is embarrassingly parallel, so may be implemented on a GPU with up to three orders of magnitude speedup.

Renjie Chen
Technion - Israel Institute of Technology
Israel
renjie.c@gmail.com

Craig Gotsman
CS dept., Technion, Israel
gotsman@cs.technion.ac.il

Kai Hormann
Università della Svizzera italiana
kai.hormann@usi.ch

MS10
Discretizing Wachspress Kernels is Safe

Barycentric coordinates were introduced by Mbius in 1827 as an alternative to Cartesian coordinates. They describe points relative to the vertices of a simplex and are commonly used to express the linear interpolant of data given at these vertices. Generalized barycentric coordinates and kernels extend this idea from simplices to polyhedra and smooth domains. In this talk, we focus on Wachspress coordinates and Wachspress kernels with respect to strictly convex planar domains. Since Wachspress kernels can be evaluated analytically only in special cases, a common way to approximate them is to discretize the domain by an inscribed polygon and to use Wachspress coordinates, which have a simple closed form. We show that this discretization, which is known to converge quadratically, is safe in the sense that the Wachspress coordinates used in this process are well-defined not only over the inscribed polygon, but over the entire original domain.

Kai Hormann
Università della Svizzera italiana
kai.hormann@usi.ch

MS10
Multi-Sided Patches and Generalized Barycentric Coordinates

This talk will review the application of generalized barycentric coordinates to multi-sided patch construction. While originally used for convex patch domains, newer generalized barycentric coordinates allow for multi-sided patches with concave domains, holes, or extensions into arbitrary dimension. We will demonstrate how to create such patches and discuss the advantages and disadvantages of this construction as well as show applications to higher dimensions such as free-form deformation.

Scott Schaefer
Texas A&M University

schaefer@cs.tamu.edu

MS10
Barycentric Coordinates for Star Polycons

Barycentric coordinates are needed in some applications for polygons with concave vertices. Such elements do not have barycentric coordinates and mean-value coordinates are widely used. Lines meeting at concave vertices may be replaced by parabolic arcs to yield polycons for which there are rational barycentric coordinates. Theoretical foundations for this option are presented in this paper. This theory has been implemented with the MATLAB program STARCON. Polygon vertices are input. Output includes barycentric coordinates for generated polycons,

Eugene L. Wachspress
Columbia University
genewac@cs.com

MS11
Quincunx Subdivision Schemes and Tight Framelets with Linear-phase Moments

Subdivision schemes with linear-phase moments have the almost interpolation property by preserving certain polynomials. In this talk, we shall introduce a family of quincunx subdivision schemes with increasing orders of sum rules and linear-phase moments while having the minimal support property and full symmetry. Such a family leads to dual quincunx subdivision schemes in CAGD. It also allows us to construct a family of symmetric tight framelets with arbitrarily high vanishing moments. The constructed symmetric quincunx subdivision schemes and tight framelets are of particular interest in computer graphics due their many desirable properties. This talk is based on the paper [B. Han, Q. Jiang, Z. Shen and X. Zhuang, Symmetric canonical quincinx tight framelets with high vanishing moments and smoothness, Mathematics of Computation, in press].

Bin Han
Univesity of Alberta
Department of Mathematical and Statistical Sciences
bhan@ualberta.ca

MS11
On the Convergence of Unstructured T-splines and Catmull-Clark Subdivision in Isogeometric Analysis

This talk presents some consolidated results on convergence evaluation of unstructured T-splines and Catmull-Clark subdivision in extraordinary regions for isogeometric analysis. The method is based on L2 projection, a set of standard geometry stencils and a class of scaled target functions, named the L2-STF method. In case of regular control meshes of bi-degree p, the method produces standard convergence rate of $p + 1$ commonly known in the literature. In case of unstructured meshes using either unstructured T-splines or Catmull-Clark subdivision, it produces the standard convergence rate in regular regions and a lower rate in extraordinary regions. The results are computed for a set of standard geometry stencils representing physical domains against a class of scaled target functions representing underlying field solutions.

Weiyin Ma
Mechanical and Biomedical Engineering
City University of Hong Kong
mewma@cityu.edu.hk

Yue Ma, Xiaoyun Yuan
City University of Hong Kong
aaron.ma@my.cityu.edu.hk, xyuan9-c@my.cityu.edu.hk

Michael Scott
Civil and Environmental Engineering
Brigham Young University
michael.scott@byu.edu

MS11
Analysis of Univariate Non-Uniform Subdivision Schemes

This paper presents a method for the analysis of convergence and smoothness of univariate non-uniform subdivision schemes. The analysis involves ideas from the theory of asymptotically equivalent subdivision schemes and non-uniform Laurent polynomial representation together with a new perturbation result. Application of the new method is presented for the analysis of interpolatory subdivision schemes based upon extended Chebyshev systems and for a class of smoothly varying schemes. (This is Joint work with N. Dyn and D. Levin.)

Jungho Yoon
Dept. Mathematics, Ewha W. Univ.,
Seoul, S.Korea
yoon@ewha.ac.kr

MS11
Subdivision Methods for Biomembranes

We present numerical methods based on subdivision methods for the well-known Canham-Evan-Helfrich model of biomembranes; and show how subdivision method occurs to be not only more accurate but also more robust than methods based on piecewise-linear surfaces. In the case of spherical surfaces, arguably the most important topology for cell biology, we develop also a flexible C^2 and higher order subdivision scheme (not available for general topology), and present experiments that suggest its superior performance over the Loop subdivision for the biomembrane problem. Along the way, we discuss also our GPU implementation of various relevant functionals, e.g. area, enclosing volume, total mean curvature, Willmore energy and harmonic energy, of subdivision surfaces. A number of open questions will be addressed.

Thomas Yu
Drexel
yut@drexel.edu

MS12
Surface Rationalization and Design for Robotic Hot-Blade Cutting

Robotic hot-blade cutting is a method for carving blocks of EPS foam with a heated rod or blade, the ends of which are controlled by a robot. As the shape of the rod can change dynamically during the movement, this allows the fast production of complex geometry for architectural formwork; however effective use of the method requires an exact and usable theoretical model in order to control the shape produced. The shape of the rod is an elastic curve segment, and hence the utilization of the technology requires surface

rationalization and/or design for surfaces foliated by elastic curves. In this talk we will present recent and ongoing work at DTU on this problem, including: (a) a method for approximating an arbitrary plane curve by an elastic curve segment using the analytic description of Eulers elastic curves in terms of elliptic functions, (b) a method for interactive modelling with elastic curves by using a special class of cubics as a proxy, and (c) an extension of this method to elastic splines.

David Brander
Technical University of Denmark
dbra@dtu.dk

MS12
Architectural Geometry in Practice

Evolute GmbH is a high-tech company founded as a spin-off from Vienna University of Technology in 2008. Since its foundation, Evolute has gained a wealth of practical expertise in enabling building projects featuring complex geometry and in solving geometric problems in automation and production technology. The paneling of freeform surfaces with panel elements of different materials and combinatorics which fulfill desired properties, such as developability and size, is one of the architectural problems Evolute specializes in. During the talk, projects from Evolute's portfolio, which revolve around such problems, will be presented. These will serve as examples of the architectural industry's recent demands for complex geometry and as the motivation behind recent advances in discrete differential geometry. Such projects include the Investcorp Building in Oxford, UK and the Eiffel Tower pavilions. New approaches to these problems and the demand for interactive tools which seamlessly incorporate the constraints imposed from these problems will also be discussed.

Konstantinos Gavriil
Evolute GmbH, Vienna
gavriil@evolute.at

MS12
Mapping Materials: Computational Methods for Material-Aware Design

In this talk I will discuss how methods from discrete differential geometry can facilitate material-aware surface design. In particular, I will show how conformal maps can be utilized to rationalize complex freeform shapes with auxetic materials, and how the theory of Chebychev nets facilitates effective algorithms for designing with wiremesh materials. I will highlight potential applications of this research in architecture, such as curved formwork and the design of static or dynamic freeform facades.

Mark Pauly
EPFL
mark.pauly@epfl.ch

MS12
Formfinding with Polyhedral Meshes

We discuss interactive modeling of polyhedral meshes for architectural design which combines form, function and fabrication, taking care of user specified constraints such as boundary interpolation, planarity of faces, panel size and shape, statics and last, but not least, cost. Our computational approach can be described as guided exploration of the constraint space whose algebraic structure is simplified

by introducing auxiliary variables and ensuring that constraints are at most quadratic. Computationally, we perform a projection onto the constraint space which is biased towards low values of an energy which expresses desirable soft properties like fairness. In particular, we present recent research on structures which use the minimal amount of material. There, we encounter remarkable relations to surfaces with minimum total absolute curvature (surface integral of the sum of absolute values of principal curvatures) and to kink angle minimizing polyhedral surfaces.

Helmut Pottmann
TU Wien
helmut.pottmann@gmail.com

MS13
Mesh Quality of Mixed-Element Bernstein-Bezier Meshes

Abstract Not Available At Time Of Publication.

Luke Engvall
CU Boulder
luke.engvall@colorado.edu

MS13
Title Not Available At Time Of Publication

Abstract Not Available At Time Of Publication.

Xifeng Gao
NYU
gxf.xisha@gmail.com

MS13
Truncated Hierarchical Box Splines in Isogeometric Analysis

Abstract Not Available At Time Of Publication.

Tadej Kanduc
Univ. Firenze
tadej.kanduc@unifi.it

MS13
Smooth Spline Spaces on Unstructured Quadrilateral and Hexahedral Meshes: Geometric Design and Isogeometric Analysis Considerations

Abstract Not Available At Time Of Publication.

Deepesh Toshniwal
UT Austin
deepesh@ices.utexas.edu

PP1
Geometrical, Algebraic, Functional, and Correlation Inequalities in Support of James-Stein Estimator for Multidimentional Projections

Isoperimetric, Milman reverse, Hilbert, Widder, Fan-Taussky-Todd, Landau, and FortuinKasteleynGinibre (FKG) inequalities in n dimensions in investigations of multidimensional estimators support the use of James-Stein estimator against classical least squares as applied to Cumulant Analysis, Associate Random Variables, and Time

Series Analysis.

Michael Fundator
Sackler Colloquium, National Academy of Sciences of USA
michaelfundator@gmail.com

PP1

Numerical Exterior Calculus Methods for Hydrodynamics Within Curved Fluid Interfaces

We develop methods based on exterior calculus of differential geometry to formulate fluctuating hydrodynamic equations to account for phenomena within curved fluid interfaces. We compare our parametrized surface methods with a Discrete Exterior Calculus approaches and Moving Least Squares solutions. We investigate rates of convergence of these methods for Laplace Beltrami Operators, Stokes Operators, as well as the Hodge Star and Exterior Derivative Operators. We also discuss application of our methods concerning physical and biological transport of inclusions (colloids, proteins) embedded within curved fluid interfaces (GUV's, lipid bilayer membranes).

Ben J. Gross, Paul Atzberger
UC Santa Barbara
bgross09@yahoo.com, atzberg@ucsb.edu

PP1

Fracture Model Reduction and Optimization for Nonlinear Flows in Porous Media

Hydraulic fracturing is a technique used in reservoir engineering to increase the productivity of oil/gas reservoirs. The properties inside the fracture is different from the porous medium. It is important to analyze the fracture geometry and model the coupled fracture porous mediua in order to explore the hydrodynamical properties of fluid flow. This work focuses on the flow filtration process of slightly compressible fluids in porous media containing fractures with complex geometries. We model the coupled fracture-porous media system where the linear Darcy flow is considered in porous media and the nonlinear Forchheimer equation is used inside the fracture. We analyze the optimal length of the fracture that maximizes the production, using the diffusive capacity, a functional that measures the performance of the reservoir. Based on methods of differential geometry, we devise a model to address the complexity of the fracture geometry. The fracture is formulated as a general surface on Riemannian manifold with the induced metric and the fracture thickness is assumed to be changing in the normal direction from the barycentric surface. Using Laplace Beltrami operator, we formulate an equation that describes the flow and then further simplifications were done. Using the model, pressure profiles of nonlinear flows are analyzed and compared with the actual pressure profiles obtained numerically in order to validate the model.

Pushpi J. Paranamana
Texas Tech University
pushpi.paranamana@ttu.edu

Eugenio Aulisa, Magdalena Toda, Akif Ibraguimov
Department of Mathematics and Statistics.
Texas Tech University
eugenio.aulisa@ttu.edu,   magda.toda@ttu.edu,
akif.ibraguimov@ttu.edu

PP1

Linear Independence of LR B-Splines

In applications such as big data compression, isogeometric analysis and geometric modeling, local refineability is an essential property for controlling the error and limiting computations. Using LR B-splines, we address progressive local refineability. This set of functions has the advantage of forming a nonnegative partition of unity and spanning the complete space of piecewise polynomials on the mesh (when the mesh construction follows certain simple rules). However, in rare cases the set of LR B-splines obtained by repeatedly splitting, throughout the construction of the mesh according to the LR-spline rules, is not linearly independent. In this work we present examples of linear dependence and discuss strategies to avoid these cases.

Francesco Patrizi
SINTEF ICT
Francesco.Patrizi@sintef.no

Tor Dokken
SINTEF ICT, Department of Applied Mathematics
Oslo, Norway
tor.dokken@sintef.no

PP1

Primitive Feature Extraction for Bivariate Spline Models

In industrial applications like computer aided design, geometric models are often represented numerically as splines or NURBS even when they originate from primitive geometry. For purposes such as redesign, it is possible to gain information about the underlying geometry through reverse engineering. In this work we combine clustering methods with approximate implicitization to determine these primitive shapes and extract their features.

Andrea Raffo
SINTEF ICT
andrea.raffo@sintef.no

Tor Dokken
SINTEF ICT, Department of Applied Mathematics
Oslo, Norway
tor.dokken@sintef.no

PP1

Manifold Charts for Point Set Surfaces

Starting from their introduction in the 19th century by Bernhard Riemann, Manifolds have proven to be tremendously useful in many applications. This also holds true for discretizations by meshes, as manifolds have been translated and applied to this setting. However, with the widespread and still growing availability of 3D scanning devices, not meshes but point clouds have become the most natural representation of real-world objects. For this data, no sound formulation of the manifold concept is available. Given a point set $P \subseteq R^3$ sampling a two-dimensional surface, we present a manifold structure defined on P that does not require meshing. This structure is equipped with local coordinate charts $\varphi : U \subseteq R^3 \to R^2$. These do not only give a two-dimensional representation of neighborhoods on the manifold, but are also enriched with structure

to allow efficient access to each point $p \in P$ and its neighborhood. Furthermore, for the intersection $U \cap V$ of the preimage of two charts φ, ψ, we present the definition of a coherent transition map $\varphi \circ \psi^{-1}$ from one coordinate chart to the other. Finally, the presented structures are applied to the setting of differential operators. We present a formulation of the point set Laplacian in terms of the structure outlined above and show that it is competitive with other Laplacians in several applications.

Martin Skrodzki
Freie University Berlin
martin.skrodzki@fu-berlin.de

Konrad Polthier
Freie Universitaet Berlin
FB Mathematik & Informatik
konrad.polthier@fu-berlin.de

PP1
Impossible NURBS via Anamorphic Deformation and Texture

Impossible objects are those that, seen from a specific vantage point, result in a (seemingly) contradictory 3D geometry. Traditionally, impossible objects are generated by taking an initial polygonal 3D model, cutting it, and deforming disconnected faces without changing their projection at the seam, so that the faces still seem adjacent from the viewpoint. We explore a more elegant approach, where we continuously deform the initial model without cuts, so that straight edges or silhouettes are still perceived as straight. The resulting geometry seems impossible because the observers assumption that the edges or silhouettes be straight is wrong. This alternative is less sensitive to displacement of the observer from the vantage point and, moreover, does not lead to gaps or texture mismatches. We show how to achieve the required deformation for NURBS-defined objects in a simple manner: just move the control points in a radial direction through the viewpoint and simultaneously change their weights. This anamorphic deformation alters the normals to the faces and hence shading. However, the introduction of textures in NURBS parameter space further deceives the eye and conceals this artifact, as the proposed deformation does not alter the projection of textures. Finally, we extend our technique in a straightforward manner, by using catoptric anamorphosis, to generate impossible views with planar mirrors.

Javier Sánchez-Reyes, Jesus M. Chacon
UCLM
Javier.SanchezReyes@uclm.es,   jesus-miguel.chacon@uclm.es

PP1
Helical Meshes Via the Cylindrical Coordinate System Graph Algorithm

The Coordinate System Graph (CSG) Algorithm is a novel technique for numerical analysis in computational geometry. The CSG algorithm is capable of generating continuous finite elements for discrete subdivision of arbitrary geometrical domains. Cartesian, cylindrical, spherical and other coordinates systems are created with the CSG algorithm. Hexahedral, quadrilateral, and one dimensional elements are rendered. The paper describes a surface and volume modeling technique which transoms a cylindrical coordinate grid into a helix. The approach will also investigate a numerical technique for computing electrostatic interactions of helical molecules using the CSG methodology. The values will be computed using a coulomb potential. The variation in gradient values are correlated to the distribution of molecular charges.

Clayton G. Thomas
Morgan State University
clayton.g.thomas@gmail.com

PP1
Find the Action of Kauffman Bracket Skein Algebra on the Skein Module of the 3-Twist Knot Complement

Kauffman bracket skein module of a 3-manifold was introduced by Jozef Przytycki[Jozef H. Przytycki, Fundamentals of Kauffman bracket skein module] as a natural generalization of the Kauffman bracket to general 3-manifolds. My current research is focused on the action of Kauffman bracket skein algebra on the skein module of the 3-twist knot complement. This is a continued work of Razvan and Nagsado's work [R.Gelca and F.Nagasato, Knot theory and its application].We consider the manifold $M = S^3 \backslash K$, where K is a 3-twist knot.We know [Bullock and Lo faro, The Kauffman bracket skein module of a twist knot exterior] $K_t(S^3 \backslash K)$ is free $C[t, t^{-1}]$-module with basis $x^k y^j$, k is arbitrary interger and j is 0,1,2,3, where $C[t, t^{-1}]$ is the ring of Laurent polynomials .We use the basis with chebyshev polynomials of second kind $S_n(x)$.Take the map $\pi : K_t(\pi^2 \times I) \rightarrow K_t(S^3 \backslash K)$.For a pair of integers (p, q), we denote by $(p, q)_T$ the element of the Kauffman bracket skein module of the 3-twist knot complement.Consider the case where $gcd(p, q) = 1$. This is the curve whose homology class in the base $(longitude, meridian)$ is (p, q).We considered curve $(1, -2)$ and $(1, -3)$ firstly to find the action of Kauffman bracket skein algebra on the skein module of these 3-twist knot complement. Eventually, we expect to find the action on a arbitrary curve using the basis with chebyshev polynomials of second kind.

Hongwei Wang
Texas Tech University
hongwei.wang@ttu.edu

Gelca Razvan
Texas Tech Univeristy
rgelca@gamil.com