List of Speakers

Plenaries:

Andy Bernoff (Harvey Mudd)

Title: Kinetic Monte Carlo Methods for Computing First Capture Time Distributions in Models of Diffusive Absorption

Abstract: Consider the pistil of a flower waiting to catch a grain of pollen, a lymphocyte waiting to be stimulated by an antigen to produce antibodies, or an anteater randomly foraging for an ant nest to plunder. Each of these problems can be modeled as a diffusive process with a mix of reflecting and absorbing boundary conditions. One can characterize the agent (pollen, antigen, anteater) finding its target (pistil, lymphocyte, ant nest) as a first passage time (FPT) problem for the distribution of the time when a particle executing a random walk is absorbed. In this talk we will examine a hierarchy of FPT problems modeling planar or spherical surfaces with a distribution of circular absorbing traps. We will describe a Kinetic Monte Carlo method that exploits exact solutions to accelerate a particle-based simulation of the capture time. A notable advantage of these methods is that run time is independent of how far from the traps one begins. We compare our results with asymptotic approximations of the FPT distribution for particles that start far from the traps. Our goal is to validate the efficacy of homogenizing the surface boundary conditions, replacing the reflecting (Neumann) and absorbing (Dirichlet) boundary conditions with a mixed (Robin) boundary condition.

This work is a collaboration with Alan Lindsay (Notre Dame) and Michael Ward (University of British Columbia).

Venkat Chandrasekaran (Caltech)

Title: Convex Graph Invariants and Their Applications

Abstract: Inverse problems over graphs arise in many application domains as graphs are widely used to model dependencies among large numbers of interacting entities; examples include gene interaction networks in computational biology, communities in social networks, and molecular structure in chemistry. To address the combinatorial complexity typically associated with such problems, we describe a conceptually unified framework based on continuous optimization for the solution of inverse problems over unlabeled graphs. Our approach is based on the notion of a convex graph invariant, which is a graph parameter that is also a convex function over the space of adjacency matrices. These invariants enable tractable algorithmic formulations for several problems on graphs and networks, most notably finding planted subgraphs and computing edit distances between graphs.

Marina Chugunova (CGU)

Title: Mathematical Modeling of Pressure Regimes in Fontan Blood Flow Circulation

Abstract: Babies born with a single functioning heart ventricle instead of the usual two require a series of surgeries during the first few years of life to redirect their blood flow. The resulting circulation, in which systemic venous blood flows directly into the pulmonary arteries, bypassing the heart, is referred to as the Fontan circulation. We develop two mathematical lumped parameter models for blood pressure distribution in the Fontan blood flow circulation: an ODE based spatially homogeneous model and a PDE based spatially inhomogeneous model. Numerical simulations of the ODE model with physiologically consistent input parameters and cardiac cycle pressure-volume outputs reveal the existence of a critical value for pulmonary resistance above which the cardiac output dramatically decreases.

Joint work with: M.G. Doyle, J.P. Keener, and R.M. Taranets

Stas Minsker (USC)

Title: Towards robust statistical learning theory

Abstract: Real-world data typically do not fit statistical models or satisfy assumptions underlying the theory exactly, hence reducing the number and strictness of these assumptions helps to lessen the gap between the “mathematical” world and the “real” world. The concept of robustness, in particular, robustness to outliers, plays the central

role in understanding this gap. Discussing the influence of outliers on statistical procedures, P. Huber observed that “..the naturally occurring deviations from the idealized model are large enough to render meaningless the traditional asymptotic optimality theory.”
In this talk, we will discuss the general principles and algorithms based on these principles that can be applied in the general framework of statistical learning theory. These algorithms avoid explicit (and often bias-producing) outlier detection and removal, instead taking advantage of induced symmetries in the distribution of the data combined with truncation.
We will discuss uniform deviation bounds for the mean estimators of heavy-tailed distributions and applications of these results to robust empirical risk minimization, in particular, the logistic regression.

The talk is partially based on a joint work with Timothée Mathieu.

Sessions:

Title: High-order, Dispersionless, Spatio-Temporally Parallel "Fast-Hybrid" Wave Equation Solver at O(1) Sampling Cost

Authors: Thomas G. Anderson

Institution: Caltech

Co-authors: Oscar Bruno, Mark Lyon

Abstract: We propose and demonstrate a frequency/time hybrid integral-equation method for the time dependent wave equation in two and three-dimensional spatial domains. Relying on Fourier Transformation in time, the method utilizes a fixed (time-independent) number of frequency-domain integral-equation solutions to evaluate, with superalgebraically- small errors, time domain solutions for arbitrarily long times. The approach relies on two main elements, namely, 1) A smooth time-windowing methodology that enables accurate band-limited representations for arbitrary long time signals, and 2) A novel Fourier transform approach which, without causing spurious periodicity effects, delivers dispersionless spectrally accurate solutions. The algorithm can handle dispersive media, complex physical structures, it enables parallelization in time in a straightforward manner, and it allows for time leaping--that is, solution sampling at any given time T at O(1)-bounded sampling cost, for arbitrarily large values of T, and without requirement of evaluation of the solution at intermediate times. The proposed frequency/time hybridization strategy, which generalizes to any linear partial differential equation in the time domain for which frequency-domain solutions can be obtained (including e.g. the time-domain Maxwell equations), provides significant advantages over other available alternatives such as volumetric discretization and convolution-quadrature approaches.

Title: Data Driven Hamiltonian Dynamics for Hydrogen-Oxygen Combustion Via Programmable Potentials

Authors: Allan Avila

Institution: University of California Santa Barbara

Co-authors: Luke Bertels, Dr. Martin Head-Gordon, Dr. Igor Mezic

Abstract: Although quantum scale simulations of hydrogen-oxygen combustion offer an accurate description of the process, a multi-atom full scale quantum level simulation of combustion would not terminate in a scientist's lifetime. Multi-atom simulations of combustion are feasible at the molecular scale, however, the potential bond energy models are often times inaccurate and results fail to match quantum simulation data. We demonstrate how to encode the coarse-level dynamical behavior into logic functions that are used to “stitch” together pairwise interaction potentials into an N-body potential. The effect of an encoding function multiplying a pairwise potential is to smoothly turn the potential on or off when a precise set of conditions are met. Our potentials are trained over sparse quantum simulation data and then inputted into a molecular dynamics simulation package (LAAMPS) for verification. Our results demonstrate that the developed programmable potentials generalize beyond the training dataset and provide a feasible manner of producing molecular level simulations for several intermediate reactions involved in hydrogen-oxygen combustion at quantum level accuracy.

Title: Bounds for the multivariate normal approximation of the group sequential maximum likelihood estimator

Authors: Julian Aronowitz

Institution: USC

Co-authors: Jay Bartroff

Abstract: Group sequential analysis is a powerful statistical framework in which sample sizes are not set before conducting a study. Instead, data is collected and analyzed in groups until the conditions of a pre-defined stopping criteria are met. A necessary factor used for determining the stopping rule in group sequential maximum likelihood estimation is the distribution of the group sequential maximum likelihood estimator (MLE). Jennison and Turnbull [1997] showed that this distribution is asymptotically multivariate normal. In this paper, we provide an optimal order Berry−Esseen type bound on the distance between the group sequential MLE and the appropriate normal distribution.

Title: "Will They Or Won't They?": Predictive Models Of Student College Commitment Decisions Using Machine Learning

Authors: Treena Basu

Institution: Occidental College

Co-authors: Ron Buckmire, Kanadpriya Basu, Nishu Lal

Abstract: Every year academic institutions invest considerable effort and substantial resources to influence, predict and understand the decision-making choices of applicants who have been offered admission. In this paper, we used four years of data on students admitted to a small liberal arts college in California to develop and test a mathematical model that predicts student college commitment decisions using several machine learning techniques. By treating the question of whether a student offered admission will accept it as a binary classification problem, we implemented a number of different classifiers and then evaluated the performance of these algorithms using the metrics of accuracy, precision, recall, F-measure and area under the receiver operator curve. The results from this study indicated that the logistic regression classifier performed best in modeling the student college commitment decision problem, i.e. predicting whether or not a student will accept an admission offer.
The significance of this research is that it demonstrates that many institutions could use machine learning algorithms to improve the accuracy of their estimates of entering class

sizes, thus allowing more optimal allocation of resources and better control over net tuition revenue.

Title: High Order Mimetic Finite Differences on Overlapping Grids

Authors: Angel Boada

Institution: San Diego State University

Co-authors: Jose Castillo

Abstract: High Order Mimetic Finite Differences based on the Mimetic Operators Divergence, Gradient and Curl have been used effectively in many applications. Overture is a portable and flexible object-oriented framework for solving partial differential equations (PDEs). One of its features is the composite overlapping grid generation for solving problems that involve the simulation of complex moving geometry. Overlapping grids are a type of block structured body-fitted conforming grids that are used to resolve fine-scale features in a particular domain. One of the most prominent advantages of using these grids is the high efficiency for high-order methods. In this talk, we examine the viability of High Order Mimetic Finite Differences on Overlapping Grids by solving representative PDEs on grids generated by Overture, while exploring different interpolation techniques on these grids (both implicitly and explicitly). Examples will be presented to demonstrate the effectiveness of the schemes.

Title: Performance improvements of Kyrlov-based solvers in numerical heat transfer and fluid flow

Authors: Matthew Blomquist

Institution: California State University Northridge

Co-authors: Abhijit Mukherjee

Abstract: In recent years, new developments in computational hardware have enabled massive parallelism that can significantly reduce the duration of computational physics simulations. However, many legacy numerical simulations are not well suited to exploit the

parallelism of modern hardware. One such example is in computational fluid dynamics, where many numerical simulations flow utilize a serial version of the Tri-Diagonal Matrix Algorithm (TDMA) to solve the linear systems that arise from the discretized equations. Krylov-based linear solvers, such as the Bi-Conjugate Gradients algorithm, can offer an ideal solution to improve the performance of these numerical simulations without requiring significant modifications to a legacy code base.

In the present work, Krylov-based linear solvers have been incorporated into a three-dimensional simulation of Rayleigh-Bénard convection. The complete, incompressible Navier-Stokes equations, along with the continuity and energy equations, are solved using SIMPLER method. The improvement in computational duration when implementing the Krylov-methods are shown against the baseline linear solver, the TDMA.

Title: Dynamic Modes of Ignition Phenomena: Learning Chemistry from Data

Authors: Cory Brown

Institution: University of California Santa Barbara

Co-authors: Ryan Mohr, Mohammad Alaghemandi, Jason R. Green, Igor Mezic

Abstract: There are no model-independent methods for the identification of the causal chemical mechanisms hidden within the emergent dynamics of ignition phenomena. Additionally, molecular dynamics simulations of atomistic models of hydrogen oxidation do not require prior knowledge of possible mechanisms or intermediates and can be validated against electronic structure calculations; along with the relative simplicity of hydrogen oxidation, this makes these simulations a natural starting point for the development of data-driven methods of analysis for both numerical simulations and experimental measurements. Here, we demonstrate a machine-learning methodology for dynamical processes, based on Koopman mode analysis, to extract dynamic modes for the kinetic stability and instability of reacting mixtures out of chemical and thermal equilibrium and apply it to extensive atomistic simulations of hydrogen oxidation. By defining persistent dynamic modes, we have developed an automated means to extract persistent local (in time) composite reactions along with a fuel-agnostic measure of ignition-delay time that correlates well with empirical measures.

Title: L_0 Structural Sparsity Regularized Convolutional Neural Networks

Authors: Kevin Bui

Institution: UC Irvine

Co-authors: Fredrick Park, Shuai Zhang, Yingyong Qi, Jack Xin

Abstract: In this work we propose a method of promoting structural sparsity in both wide and deep convolutional neural networks. Deepening and widening the the network significantly increases the number of trainable parameters by respectively adding more convolutional layers and adding more feature maps in each layer. Imposing structural sparsity prunes groups of neurons during the training process which accelerates the training and systematically compresses networks. The remaining groups in these compressed networks also possess intra-group sparsity. These attributes allow for networks to avoid over-fitting while also having significantly faster inference speeds. In order to promote such structured sparsity in convolutional neural networks, we regularize the network weights by incorporating ℓ_0 into the loss function. To address the non-differentiability of this norm, we apply a relaxed variable splitting method with thresholding that is compatible with stochastic gradient descent. We also show how this method can be applied to relaxed variants of the ℓ_0 norm in the ℓ_1 and transformed-ℓ_1 norms. Numerical experiments are demonstrated on residual neural networks and wide residual networks, showcasing the effectiveness of our proposed method in network sparsification and test accuracy on par with the current state of the art.

Title: A Discontinuous Galerkin Method for the Aw-Rascle Traffic Flow Model on Networks

Authors: Josh Buli

Institution: University of California, Riverside

Co-authors: Yulong Xing

Abstract: In this talk we consider the second-order Aw-Rascle (AR) model for traffic flow on a network, and propose a discontinuous Galerkin (DG) method for solving the AR system of hyperbolic PDEs with appropriate coupling conditions at the junctions. For the proposed method we apply the Lax-Friedrichs flux, and for comparison, we use the first-order Lighthill-Whitham-Richards (LWR) model with the Godunov flux. Coupling conditions are also required at the junctions of the network for the problem to be well-posed. As the choice of coupling conditions is not unique, we test different coupling conditions for the Aw-Rascle model at the junctions. Numerical examples are provided to demonstrate the high-order accuracy, as well as comparisons between the first-order LWR model and the second-order AR model. The ability of the AR model to capture the capacity drop phenomenon is also explored.

Title: Data-driven multiscale modeling of the role of signaling in the maintenance of transcription factor distribution in stem cell homeostasis

Authors: Weitao Chen

Institution: University of California, Riverside

Co-authors: Venugopala Gonehal, Mark Alber

Abstract: The regulation and interpretation of transcription factor levels is critical in spatiotemporal regulation of gene expression in development biology. However, concentration-dependent transcriptional regulation, and the spatial regulation of transcription factor levels are poorly studied in plants. WUSCHEL, a stem cell-promoting homeodomain transcription factor was found to activate and repress transcription at lower and higher levels respectively. The differential accumulation of WUSCHEL in adjacent cells is critical for spatial regulation on the level of CLAVATA3, a negative regulator of WUSCHEL transcription, to establish the overall gradient. Experiments show that subcellular partitioning and protein destabilization control the WUSCHEL protein level and spatial distribution. Meanwhile the destabilization of WUSCHEL also depends on the protein concentration which in turn is influenced by intracellular processes. However, the roles of extrinsic spatial cues in maintaining differential accumulation of WUSCHEL are not well understood. We develop a 3D cell-based mathematical model which integrates sub-cellular partition with cellular concentration across the spatial domain to analyze the regulation of WUS. By using this model, we investigate the machinery of the maintenance of WUS gradient within the tissue. We also developed a hybrid ODE mathematical model

of stochastic binding and unbinding of WUS to cis-elements regulating CLV3 expression, connected with deterministic dynamics that accounts for WUS protein dynamics to understand the concentration dependent manner mechanistically. By using the hybrid model, we can explore hypotheses regarding the nature of co-operative interactions among cis-elements, the influence of WUS complex stoichiometry (monomer versus dimer binding) on the transcriptional switching behavior and the CLV3 signaling feedback on the regulation of WUS protein levels, which is critical for stem cell homeostasis.

Title: PDE models for sizer, timer, and adder mechanisms of cellular proliferation

Authors: Tom Chou

Institution: UCLA

Co-authors: Mingxia Tao, Chris Greenman

Abstract: Cell division is a process that involves many biochemical steps and complex biophysical mechanisms. To simplify the understanding of what triggers cell division, three basic models that subsume more microscopic cellular processes associated with cell division have been proposed. Cells can divide based on the time elapsed since their birth, their size, and/or the volume added since their birth - the timer, sizer, and adder models, respectively. While the populations of cells dividing under sizer and timer rules have been treated individually, we develop a unified PDE model that incorporates all mechanisms, especially that of the adder. Limiting cases of our model reduce to single-mechanism models previously proposed. Specifically, we show that the adder mechanism is not independent of the timer mechanism under deterministic cell growth; however, our adder model provides an easier way to incorporate mechanisms in terms of added volume and exhibit qualitatively different dynamical behavior. We further generalize our PDE model to incorporate mother-daughter correlations in cellular growth rates. Existence and uniqueness of weak solutions to our PDE model are proved, allowing us to numerically compute the dynamics of cell population densities. Finally, we carry out numerical studies to illustrate blow-up of the average cell size and evolution of cellular growth rates.

Title: A Riemannian Optimization of Correlation Matrices

Authors: Paul David

Institution: Claremont Graduate University

Co-authors: Weiqing Gu

Abstract: The set of non-degenerate correlation matrices $Corr(n)$ is described in terms of a newly found Riemannian quotient structure arising from a group action on the manifold of symmetric positive-denite matrices $SPD(n)$. The key characterizations of $SPD(n)$ as a homogeneous space are naturally inherited by $Corr(n)$ deepening the geometric relationship between nondegenerate covariances and correlations. In particular the affine-invariant metric on $SPD(n)$, regarded as a canonical metric on this space, exhibits great symmetry with the quotient structure of $Corr(n)$ allowing for straightforward computations of geodesics and distances on this manifold. We subsequently develop a Riemannian Newton's optimization procedure on $Corr(n)$, making full use of its quotient manifold structure, involving iterations between $Corr(n)$ and its ambient manifold $SPD(n)$. The Newton method is then evaluated in terms of reconstruction errors, convergence and run time, and is also applied to problems in unsupervised anomaly detection and person identification.

Title: Convergence of a Relaxed Variable Splitting Method for Learning Sparse Neural Networks via l_1, l_0, and transformed-l_1 Penalties

Authors: Thu Dinh

Institution: UC Irvine

Co-authors: Jack Xin

Abstract: Sparsification of neural networks is one of the effective complexity reduction methods to improve efficiency and generalizability. We consider the problem of learning a one hidden layer convolutional neural network with ReLU activation function via gradient descent under sparsity promoting penalties. It is known that when the input data is Gaussian distributed, no-overlap networks (without penalties) in regression problems with ground truth can be learned in polynomial time at high probability. We propose a relaxed variable splitting method integrating thresholding and gradient descent to overcome the

lack of non-smoothness in the loss function. The sparsity in network weight is realized during the optimization (training) process. We prove that under $\ell 1, \ell 0$; and transformed-$\ell 1$ penalties, no-overlap networks can be learned with high probability, and the iterative weights converge to a global limit which is a transformation of the true weight under a novel thresholding operation. Numerical experiments confirm theoretical findings, and compare the accuracy and sparsity trade-off among the penalties.

Title: An Adaptive Bounding Subgradient Optimization Algorithm

Authors: Nicholas Dwork

Institution: University of California, San Francisco

Co-authors: Charles Tsao, Jorge Balbas, Cody Coleman, John Pauly

Abstract: We present a subgradient optimization method with a novel strategy to adapt the step size of successive iterations based on the recent history of the trajectory. The proposed algorithm accelerates the rate of convergence of subgradient optimization for non-differentiable objective functions. Along with a detailed description of the method, we prove its convergence for convex optimization problems and validate its performance by solving several examples arising from relevant applications ranging from scalar problems to the training of a neural network for image classification (a non-convex problem). The comparison of the proposed method to well established optimization algorithms demonstrates its robustness and suitability for optimizing non-differentiable objective functions.

Title: A mechanistic model for embryonic lung morphogenesis

Authors: Uduak Z. George

Institution: San Diego State University

Co-authors: Sharon R. Lubkin

Abstract: This talk presents our recent findings on lung branching morphogenesis. Lung branching morphogenesis proceeds in three stereotyped modes (domain, planar, and orthogonal branching). Much is known about the molecular players, including growth factors such as fibroblast growth factor 10 but it is unknown how these signals could actuate the different branching patterns. With the aim of identifying mechanisms that may determine the different branching modes, we developed a computational model of the epithelial lung bud and its surrounding mesenchyme. We studied transport of morphogens and localization of morphogen flux at lobe surfaces and lobe edges using partial differential equations. Our simulation results show that the elongation, bending, flattening, or bifurcation of epithelial tubule depends solely on geometric ratios of the tissues in the vicinity of a growing tubule tip. Furthermore, the same simple mechanism of geometric ratios is capable of generating orthogonal or planar branching.

Title: A wave of locusts

Authors: Maryann Hohn

Institution: UC Santa Barbara

Co-authors: Andrew Bernoff, Michael Culshaw-Maurer, Rebecca Everett, Christopher Strickland, and Jasper Weinburd

Abstract: Juvenile locusts gather together and march through fields in a hopper band. By doing so, they form a wave of advancing insects which we examined in two ways: using an agent-based model and a set of partial differential equations. The agent-based model is based on observations of individual locust behavior from biological data while the PDE gives insight into collective behavior of the front of the band of locusts. In this poster, we will present the creation of the models and how we can determine the speed of the wave of locusts and the amount of food left behind.

Title: Locating the Source of Large-Scale Diffusion of Foodborne Contamination

Authors: Abigail Horn

Institution: USC

Co-authors: Hanno Friedrich

Abstract: During a large-scale outbreak of foodborne disease, rapidly identifying the source, including both the food vector carrying the contamination and the location source in the supply chain, is essential to minimizing the impact on public health and industry. However, tracing an outbreak to its origin is a challenging problem due to the complexity of the food supply system and the absence of publicly available data on the fine-grained structure of the intra-company supply chain.

In this talk I will present a framework we have developed that integrates novel modeling techniques with nontraditional data sources to identify the source of emerging outbreaks of foodborne disease. Approaching this problem requires (i) modeling the network structure of the aggregated food supply system and (ii) developing network-theoretic methods to identify the food vector carrying the contamination and the location source in the supply network. I will discuss our approach to both parts of this problem, experiences implementing these methods at Germany's federal-level food regulatory agency, and a developing project to extend this work to the US context.

First, I will introduce our approach to model the network structure of the aggregated food supply system utilizing publicly available statistical data and methods from transport demand modeling [1]. Then I will review our network epidemiological approach to identify the food and location source of an outbreak given the food supply network model and reported locations of illness [2,3]. To solve the source location problem we formulate a probabilistic model of the contamination diffusion process and derive the maximum likelihood estimator for the source location. We use the location source estimator as the basis of an information-theoretic approach to identify the food vector source carrying the contamination. A statistical test is developed to identify the food item network that best fits the observed distribution of illness data.

Case studies on several recent outbreaks in Germany suggest that the application of the combined network models and inference methods could have substantial benefits for investigators during the onset of large-scale outbreaks. Beyond foodborne disease, we are applying these methods to identify the source of network-based diffusion processes more generally, including infectious diseases spread through the global air mobility networks and cholera spread through water distribution networks.

[1] Balster, A., and Friedrich, H. (2018). "Dynamic freight flow modelling for risk evaluation in food supply," Transportation Research E, https://doi.org/10.1016/j.tre.2018.03.002.
[2] Horn, A., Friedrich, H. (2019). Locating the source of large-scale outbreaks of

foodborne disease. J. R. Soc. Interface 16: 20180624.
http://dx.doi.org/10.1098/rsif.2018.0624
[3] Horn, A., Friedrich, H., Balster, B., Polozova, E., Fuhrmann, M., Weiser, A., Kaesbohrer, A., and Filter, M. (2018). “Identifying Food and Location Origin of Large-scale Outbreaks of Foodborne Disease.” in prep.

Title: Consistency of semi-supervised learning algorithms

Authors: Bamdad Hosseini

Institution: Caltech

Co-authors: Franca Hoffmann, Zhi Ren, Andrew Stuart

Abstract: Graphical semi-supervised learning is the problem of labelling the vertices of a graph given the labels of a few vertices along with geometric information about the graph. Such problems have attracted a lot of attention in machine learning for classification of large datasets. In this talk we discuss consistency and perturbation properties of the probit and one-hot methods for semi-supervised learning. We show that, under certain conditions, both methods result in a unique solution that predicts the correct label of all of the vertices.

Title: A Fast Hierarchically Preconditioned Eigensolver Based on Multiresolution Matrix Decomposition

Authors: De Huang

Institution: Caltech

Co-authors: Thomas Y. Hou, Kachun Lam, Ziyun Zhang

Abstract: In this work we propose a new iterative method to hierarchically compute a relatively large number of leftmost eigenpairs of a sparse symmetric positive matrix under the multiresolution operator compression framework. We exploit the well-conditioned property of every decomposition components by integrating the multiresolution framework

into the Implicitly Restarted Lanczos method. We achieve this combination by proposing an extension-refinement iterative scheme, in which the intrinsic idea is to decompose the target spectrum into several segments such that the corresponding eigenproblem in each segment is well-conditioned. Theoretical analysis and numerical illustration are also reported to illustrate the efficiency and effectiveness of this algorithm.

Title: Stefan problems with flow: Dissolution of a candy ball

Authors: Jinzi Mac Huang

Institution: UCSD

Abstract: Natural convection accompanies many Stefan problems such as the dissolution and melting of solid objects in fluid. Gravity driven flows are responsible for many land-forming processes, for example the formation of Karst landscapes and the "stone forests" of China and Madagascar. Smaller structures, like iceberg "scallops", are also a consequence of natural convection. Recent experimental results show that even much simpler cases of dissolution of a spherical candy can lead to very nontrivial pattern formation. In this talk, we will present a numerical study of fluid-coupled Stefan problems, based on a high-order Immersed Boundary Smooth Extension method for evolving the boundaries of soluble solids immersed in a fluid. The method yields solutions with high regularity across boundaries, which allows us to evolve the geometry with high order of accuracy. The generated solution bears close resemblance to the shape of dissolved candy, where non-smooth patterns form at the bottom surface of candy.

Title: Wavelet algorithms for a high-resolution image reconstruction in magnetic induction tomography

Authors: Ahmed Kaffel

Institution: Marquette University

Abstract: Electrical conductivity (EC) varies considerably throughout the human body. Thus, an ability to image its spatial variability could be useful from a diagnostic standpoint. Various disease states may cause the conductivity to differ from that exhibited

in normal tissue. EC imaging in the human body is usually pursued by either electrical impedance tomography or magnetic induction tomography (MIT).
Nearly all MIT work uses a multiple coil system. More recently, MIT has explored using a single coil, whose interaction with nearby conductive objects is manifested as an inductive loss. This work has shown that single-coil, scanning MIT is feasible through an analytical 3D convolution integral that relates measured coil loss to an arbitrary conductivity distribution and permits image reconstruction by linear methods.
The convolution integral must be discretized over a space that includes the target, a step currently achieved using finite elements. Though feasible, it has major drawbacks, primarily due to the need to know target boundaries precisely. Here, we propose to discretize the convolution integral using wavelets, with a goal of alleviating the problem of unknown boundaries and providing spatial resolving power where it is most needed in the target domain.

Title: Volume preserving mean curvature flow for star-shaped sets

Authors: Dohyun Kwon

Institution: University of California, Los Angeles

Co-authors: Inwon Kim

Abstract: Mean curvature flows appear in many physical applications such as material science and image processing. The evolution of convex sets for motion by mean curvature including anisotropic or crystalline one has been well-studied. In this talk, we present the evolution of star-shaped sets in volume preserving mean curvature flow. Constructed by mean curvature flows with forcing and their minimizing movements, our solution preserves a strong version of star-shapedness for all time. We use the gradient flow structure of the problem and show that the solutions converges to a ball as time goes to infinity. This is a joint work with Inwon Kim.

Title: Nonparametric Estimation of a Mixing Distribution for Pharmacokinetic Stochastic Models

Authors: Alona Kryshchenko

Institution: California State University of Channel Islands

Co-authors: Alan Schumitzky, Mike van Guilder, Michael Neely

Abstract: We develop a nonparametric maximum likelihood estimate of the mixing distribution of the parameters of a linear stochastic dynamical system. This includes, for example, pharmacokinetic population models with process and measurement noise that are linear in the state vector, input vector and the process and measurement noise vectors. Most research in mixing distributions only considers measurement noise. The advantages of the models with process noise are that, in addition to the measurements errors, the uncertainties in the model itself are taken into the account. For example, for deterministic pharmacokinetic models, errors in dose amounts, administration times, and timing of blood samples are typically not included. For linear stochastic models, we use linear Kalman-Bucy filtering to calculate the likelihood of the observations and then employ a nonparametric adaptive grid algorithm to find the nonparametric maximum likelihood estimate of the mixing distribution.

Title: Fast Optimal Transport

Authors: Flavien Leger

Institution: UCLA

Co-authors: Matt Jacobs

Abstract: We present a method to efficiently solve the optimal transportation problem for a general class of strictly convex costs. Given two probability measures supported on a discrete grid with n points we compute the optimal transport map between them in $O(nlog(n))$ operations and $O(n)$ storage space. Our approach allows us to solve optimal transportation problems on spatial grids as large as 4096 x 4096 and 256 x 256 x 256 in less than 3 minutes on a personal computer even before applying parallelization or other scientific computing techniques.

Title: Modeling the Effects of Vector-Induced Responses on Pathogen Transmission Between Hosts

Authors: Jing Li

Institution: California State University Northridge

Co-authors: David Crower, Evan Habbershaw, Jeb Owen

Abstract: Plant disease is often transmitted among plants by an infectious agent called a vector during the process of vector feeding on plants. As a result of insect feeding without a pathogen, there are already interactions between plants and vectors, which have a variety of effects, including a reduction in nutrient acquisition and vector fitness, and an increase in vector movement, etc. Most of these interactions are considered as the vector-induced host defensive responses against the vectors. We investigate how such responses affect the spread of a vector-borne pathogen in the host population, using compartmental models. We incorporate the responses into the model by introducing separate compartments for vector-susceptible and vector-refractory plant hosts. A stability analysis is performed along with a thorough sensitivity analysis to investigate the effects of vector-induced host responses on disease spread. Numerical simulations are performed to verify the results found in the stability and sensitivity analyses. The sensitivity analysis indicates that vector-induced defensive host responses are important factors impacting the spread of a pathogen in a plant disease system. Changes in feeding rates have a substantial effect, positively correlating with the disease spread. Changes in transmission probabilities also have a significant impact; a lowered transmission probability corresponds to a slower pathogen spread. The proportion of vector refractory hosts in a population at the onset of a disease is also essential to influence pathogen spread; a higher percentage of vector refractory hosts leads to a lower growth rate of the pathogen in the system. Such a finding implies that allowing vectors to feed and remain on uninfected plant hosts potentially slows down the disease spread. Therefore, it is practically advisable not to completely remove the insect population from host plants to prevent disease spread.

Title: Learning graph structure from linear measurements: Fundamental tradeoffs and application to electric grids

Authors: Tongxin Li

Institution: Caltech

Co-authors: Lucien Werner, Steven H. Low

Abstract: We consider a specific graph learning task: reconstructing a symmetric matrix that represents an underlying graph using linear measurements. We study fundamental tradeoffs between the number of measurements (sample complexity), the complexity of the graph class, and the probability of error by first deriving a necessary condition (fundamental limit) on the number of measurements. Then, by considering a two-stage recovery scheme, we give a sufficient condition for recovery. Furthermore, assuming the measurements are Gaussian IID, we prove upper and lower bounds on the (worst-case) sample complexity. In the special cases of the uniform distribution on trees with n nodes and the Erdos-Renyi (n,p) class, the fundamental trade-offs are tight up to multiplicative factors. In addition, we design and implement a polynomial-time (in n) algorithm based on the two-stage recovery scheme. Simulations for several canonical graph classes and IEEE power system test cases demonstrate the effectiveness of the proposed algorithm for accurate topology and parameter recovery.

Title: Learning via Wasserstein information geometry

Authors: Wuchen Li

Institution: UCLA

Co-authors: Alex Lin, Guido Montufar, Stanley Osher

Abstract: In this talk, I start with reviewing several differential structures from optimal transport (Wasserstein metric). Based on it, I will introduce the Wasserstein natural gradient in parametric models. The L2-Wasserstein metric tensor in probability density space is pulled back to the one on parameter space, under which the parameter space forms a Riemannian manifold. The Wasserstein gradient flows and proximal operator in parameter space are derived. We demonstrate that the Wasserstein natural gradient works efficiently in several machine learning examples, including Boltzmann machines and generative adversary models (GANs).

Title: Acceleration of Primal-Dual Methods by Preconditioning and Simple Subproblem Procedures

Authors: Yanli Liu

Institution: UCLA

Co-authors: Yunbei Xu, Wotao Yin

Abstract: Primal-Dual Hybrid Gradient (PDHG) and Alternating Direction Method of Multipliers (ADMM) are two widely-used first-order optimization methods. They reduce a difficult problem to simple subproblems, so they are easy to implement and have many applications. As first-order methods, however, they are sensitive to problem conditions and can struggle to reach the desired accuracy. To improve their performance, researchers have proposed techniques such as diagonal preconditioning and inexact subproblems. This paper realizes additional speedup about one order of magnitude.

Specifically, we choose non-diagonal preconditioners that are much more effective than diagonal ones. Because of this, we lose closed-form solutions to some subproblems, but we found simple procedures to replace them such as a few proximal-gradient iterations or a few epochs of proximal block-coordinate descent, which are in closed forms. We show global convergence while fixing the number of those steps in every outer iteration. Therefore, our method is reliable and straightforward.

Our method opens the choices of preconditioners and maintains both low per-iteration cost and global convergence. Consequently, on several typical applications of primal-dual first-order methods, we obtain $4--95\times$ speedup over the existing state-of-the-art.

Title: Dimension-Reduced Dynamics From Slow-Fast Systems Using Diffusion Kernels

Authors: Krithika Manohar

Institution: Caltech

Co-authors: Dimitris Giannakis, Andrew Stuart

Abstract: Complex systems with dynamics evolving on multiple timescales pose a tremendous challenge for data analysis and modeling. In practice, complex systems such as oceans and climate, when they exhibit clear scale separation, are often modeled by treating fast variables as stochastic or noise effects. Kernel algorithms in machine learning

are powerful modeling tools that provide data-driven approximations of operators governing the macroscopic observables for these systems. We apply diffusion kernels to a deterministic slow-fast system that resembles a lower-dimensional SDE in the slow variable. The resulting diffusion eigenvectors computed from the deterministic slow variable are shown to approximate the analytic Laplace-Bertrami eigenfunctions of the lower-dimensional SDE. Using these eigenfunctions as a basis, we construct an operator semigroup modeling the slow dynamics, and study its predictive skill.

Title: Nonspecific Probe Binding and Automatic Gating of Cell Identification in Flow Cytometry

Authors: Bhaven Mistry

Institution: UCLA

Co-authors: Tom Chou

Abstract: Flow cytometry is extensively used in cell biology to differentiate cells of interest (mutants) from control cells (wild-types). For mutant cells characterized by expression of a distinct membrane surface structure, fluorescent marker probes can be designed to bind specifically to these structures while the cells are in suspension, resulting in a sufficiently high fluorescence intensity measurement by the cytometer to identify a mutant cell. However, cell membranes may have relatively weak, nonspecific binding affinity to the probes, resulting in false positive results. Furthermore, the same effect would be present on mutant cells, allowing both specific and nonspecific binding to a single cell. We derive and analyze a kinetic model of fluorescent probe binding dynamics by tracking populations of mutant and wild-type cells with differing numbers of probes bound specifically and nonspecifically. By assuming the suspension is in chemical equilibrium prior to cytometry, we use a two-species Langmuir adsorption model to analyze the confounding effects of non-specific binding on the assay. Furthermore, we analytically derive an expectation maximization method to infer an appropriate estimate of the total number of mutant cells as an alternative to existing, heuristic methods. Lastly, using our model, we propose a new method to infer physical and experimental parameters from existing protocols. Our results provide improved ways to quantitatively analyze flow cytometry data.

Title: Application of Transfer Matrix Method, Green's Function, and Galerkin Theory to Predict Diffuse Absorption Coefficient

Authors: Duyen Nguyen (undergrad)

Institution: California State University, Long Beach

Co-authors: Allen Teagle-Hernandez

Abstract: Acoustic calculations that use the Transfer Matrix Method (TMM) occasionally underestimate the sound absorption performance of multi-layered porous material when compared to experimentally obtained data. This is especially true when the experimental data pertains to reverberant (Diffuse-Sabine) absorption. Additionally, when there is a large impedance mismatch between the reverberant wall and the porous specimen, experimental data indicates Absorption Coefficients greater than 1, which defies the law of conservation of energy. It is hypothesized that the extra absorption is due to the diffraction of waves occurring at the edge of the tested materials, thus increasing the area where energy is being absorbed. This contradiction of the law of energy is often referred to as the “edge effect”. The purpose of this research is to predict the edge effect within reverberation and anechoic rooms by using Green’s function and Boundary Integral technique. A Galerkin approach is used to obtain the normalized radiation impedance.

Title: A Model of Thrombus Compression Mediated by Thrombocytes Contractile Forces

Authors: Francesco Pancaldi

Institution: University of California Riverside

Co-authors: Samuel Britton, Oleg Kim, Zhiliang Xu, Rustem I. Litvinov, John W. Weisel, Mark Alber

Abstract: Blood clots are fundamental bio-material structures formed as a result of the coagulation cascade initiated by injuries and inflammation aimed to contain hemorrhagic events in damaged blood vessels. The integrity and stability of these thrombi are fundamental in order to avoid coagulation related pathologies such as stroke, deep vein thrombosis, and uncontrolled bleeding. In this study, we are improving on our previously developed computational fibrin network mechanical model [1] introducing activated

platelet cells and the contractile forces induced by their tendrils on the blood clot. We first compare the resulting computational clots contraction with experimental results and then, through computational simulations, we show how different factors including density of platelets, distribution of platelets, and contractile forces, result in different compression dynamics for the simulated thrombus.

[1] E. Kim, O.V. Kim, K.R. Machlus, X. Liu, T. Kupaev, J. Lioi, A.S. Wolberg, D.Z. Chen, E.D. Rosen, Z. Xu, M. Alber, Correlation between fibrin network structure and mechanical properties: an experimental and computational analysis, Soft Matter. 7 (2011) 4983–4992.

Title: Quasi-Newton Optimization For Large-scale Machine Learning

Authors: Jacob Rafati

Institution: University of California, Merced

Co-authors: Roummel F. Marcia

Abstract: Deep learning algorithms often require solving a highly non-linear and nonconvex unconstrained optimization problem. Methods for solving the optimization problems in large-scale machine learning, deep learning and deep reinforcement learning (RL) are restricted to the class of first-order algorithms, like stochastic gradient descent (SGD). The major drawback of the SGD methods is that they have the undesirable effect of not escaping saddle-points. Furthermore, these methods require exhaustive trial-and-error to fine-tune many learning parameters. Using second-order curvature information to find search directions can help with more robust convergence for non-convex optimization problems. However, computing Hessian matrices for large-scale problems is not computationally practical. Alternatively, quasi-Newton methods construct an approximate of the Hessian matrix to build a quadratic model of the objective function. Quasi-Newton methods, like SGD, require only first-order gradient information, but they can result in superlinear convergence, which makes them attractive alternatives to SGD. The limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) approach is one of the most popular quasi-Newton methods that construct positive definite Hessian approximations. In our research, we have proposed efficient optimization methods based on L-BFGS quasi-Newton methods using line search and trust-region strategies. Our method bridges the disparity between first order methods and second order methods by using

gradient information to calculate low-rank updates to Hessian approximations. We have studied formal convergence analysis as well as empirical results on variety of the large-scale machine learning tasks, such as image classification tasks, and deep reinforcement learning on classic ATARI 2600 games. Our results show a robust convergence with preferred generalization characteristics as well as fast training time.

Title: Asymptotically consistent algorithms for clustering covariance stationary ergodic processes

Authors: Nan Rao

Institution: Claremont Graduate University

Co-authors: Qidi Peng, Ran Zhao

Abstract: Covariance stationary processes have wider applications than distribution stationary processes. In this framework we introduce and study the problems of clustering covariance stationary ergodic processes. A new covariance-based dissimilarity measure is presented, from which efficient asymptotically consistent clustering algorithms are designed. In a simulation study, several excellent examples are provided to show the efficiency and consistency of the clustering algorithms. Comparison to the other existing clustering algorithms is made. In a real world project, we successfully apply these algorithms to cluster the global equity markets of different regions.

Title: Iterative linear solvers and random matrices: new bounds for the block Gaussian sketch and project method

Authors: Elizaveta Rebrova

Institution: University of California Los Angeles

Co-authors: Deanna Needell

Abstract: One of the most famous methods for solving large-scale over-determined linear systems is Kaczmarz algorithm, which iteratively projects the previous approximation onto the solution space of the next equation in the system. Sketch and project framework

(due to Gower and Richtarik) is a unifying view on a number of iterative solvers, including Kaczmarz. Its main idea is as follows: one can observe that the random selection of the next projection direction can be represented as a sketch, that is, left multiplication by a certain random vector (or a matrix). In particular, this gives an idea to study a broader class of Kaczmarz-type methods, represented by new sketch types.
In our work with Deanna Needell, we study the case when every sketch is given by a gaussian random matrix (one of the best-understood models in the random matrix theory). We were able to employ some random matrix theory results and concentration of measure ideas to prove fast convergence and improved behavior in the presence of noise of this block Gaussian sketch and project method.

Title: Exact Importance Sampling of Affine Processes

Authors: Alex Shkolnik

Institution: University of California, Santa Barbara

Abstract: Affine processes are ubiquitous in finance due to their rich behavior and mathematical tractability. But for tail computations in a multivariate setting, this tractability has its limits. Importance sampling (IS) algorithms are a class of Monte Carlo methods to solve such tail estimation problems. However, a standard IS scheme entails an exponential change of measure (ECM) under which the affine process acquires a time-dependent drift. This prohibits exact sampling. We circumvent this problem by introducing an approximate ECM under which the drift coefficient is a step function. This permits exact sampling of the affine jump-diffusion skeleton under the proposed importance measure. As the (skeleton) discretization shrinks, the limiting measure coincides with that of the ECM and inherits all of its optimality properties. We illustrate the advantage of this exact importance sampling algorithm on a pricing application.

Title: The conjugate gradient algorithm on random matrices

Authors: Tom Trogdon

Institution: UC Irvine

Co-authors: Percy Deift, Govind Menon

Abstract: Numerical analysis and random matrix theory have long been coupled, going (at least) back to the seminal work of Goldstine and von Neumann (1951) on the condition number of random matrices. The works of Trotter (1984) and Silverstein (1985) incorporate "numerical techniques" to assist in the analysis of random matrices. One can also consider the problem of computing distributions (i.e. Tracy-Widom) from random matrix theory. In this talk, I will discuss a different numerical analysis problem: using random matrices to analyze the runtime (or halting time) of numerical algorithms. I will focus on recent results for the conjugate gradient algorithm including a proof that the halting time is almost deterministic.

Title: Post-treatment control of HIV infection under conditioning of drugs of abuse

Authors: Peter Uhl

Institution: San Diego State University

Co-authors: Naveen K. Vaidya

Abstract: Despite tremendous successes of antiretroviral therapy (ART), there is no cure for HIV, in part due to establishment of latently infected cells, which often result in viral rebounds (VR) after the therapy is stopped. However, recent studies suggest that some patients, depending on latent reservoir size and the strength of the cellular immune response, can maintain viral load below the detection limits even after the treatment termination, exhibiting post-treatment control (PTC). Importantly, both latent reservoir size and cellular immune response are highly affected by the presence of drugs of abuse. In this study, we develop a mathematical model to study how the presence of drugs of abuse (morphine) can influence the post-treatment dynamics of HIV. Our model predicts that morphine conditioning can make it more likely a patient will undergo VR by increasing the immune strength required to maintain PTC. Using our model, we also identify that the time to VR is significantly decreased by the presence of morphine in the body.

Title: Porous Medium Equation with a Drift: Free Boundary Regularity

Authors: Yuming Zhang

Institution: UCLA

Co-authors: Inwon Kim

Abstract: We study regularity properties of the free boundary for solutions of the porous medium equation with the presence of drift. First, if the initial data has super-quadratic growth at the free boundary, then the support strictly expands relative to the streamline. We then proceed to show the nondegeneracy and $C^{1,\alpha}$ regularity of the free boundary, when the solution is directionally monotone in space variable in a local neighborhood. The main challenge lies in establishing a local non-degeneracy estimate, which appears new even for the zero drift case.

Title: On The Worst-case Sensitivity of Optimal Power Flow Problems

Authors: Fengyu Zhou

Institution: Caltech

Co-authors: James Anderson, Steven H. Low

Abstract: Optimal power flow problems (OPFs) are mathematical programs used to distribute power over networks subject to network operation constraints and the physics of power flows. In this work we take the view of treating an OPF problem as an operator which maps user demand to generated power and allow the network parameters to take values in some admissible set. The contributions of this paper are to formalize this operator approach, define a sensitivity metric of the operator taken as the worst-case over the admissible set, and characterize the computational complexity of such a problem. We show that the resulting mathematical program in general is a non-convex combinatorial optimization problem. However, under three types of network topologies (tree, uni-cyclic graph and the graph with multiple non-adjacent cycles), the structural properties of the problem make it possible to efficiently calculate the worst-case sensitivity. Our results also provide insights for related applications such as data privacy in power systems, real-time OPF computation, and locational marginal price.