Plenary Talks

Approximation of advection-diffusion equations using implicit WENO methods
Todd Arbogast, University of Texas at Austin

Abstract: Within the life sciences, researchers use models that often involve advective, diffusive, and reactive processes. These are often formulated as systems of nonlinear advection-diffusion-reaction equations. These equations are often advection dominated; moreover, the diffusion may degenerate (to zero). This means that the solutions to the equations can and often do develop steep fronts or even shock discontinuities. We consider approximation of nonlinear advection-diffusion equations using finite volume methods. These methods require two components: (1) reconstruction of a function from knowledge of its element averages and (2) time stepping (in the sense of the method of lines). We first discuss function reconstruction using the weighted essentially non oscillatory (WENO) framework, which allows accurate reconstruction of function values near function discontinuities. We develop a multi-scale, WENO method with adaptive order (WENO-AO), and analyze its performance theoretically and computationally. The idea is to create a high order accurate reconstruction where the function is smooth, and drop the order of the approximation and bias the reconstruction stencil to one side of a discontinuity. We next discuss time stepping procedures of the implicit type, because advection-diffusion equations are stiff. High order Runge-Kutta (RK) methods can fail near discontinuities (i.e., generate oscillations), so we develop a hybrid approach combining the RK method with a simple and stable backward Euler (BE) method. Finally, we discuss approximation of degenerate diffusion within the finite volume WENO framework.

Modeling the chemotherapy-induced selection of drug-resistant traits during tumor growth
Doron Levy, University of Maryland

Abstract: The emergence of drug-resistance is a major challenge in chemotherapy. In this talk we will present our recent mathematical models for describing the dynamics of drug-resistance in solid tumors. Our models follow the dynamics of the tumor, assuming that the cancer cell population depends on a phenotype variable that corresponds to the resistance level to a cytotoxic drug. We incorporate the dynamics of nutrients and two different types of drugs: a cytotoxic drug, which directly impacts the death rate of the cancer cells, and a cytostatic drug that reduces the proliferation rate. Through analysis and simulations, we study the impact of spatial and phenotypic heterogeneity on the tumor growth under chemotherapy. We demonstrate that heterogeneous cancer cells may emerge due to the selection dynamics of the environment. Our models predict that under certain conditions, multiple resistant traits emerge at different locations within the tumor. We show that a higher dosage of the cytotoxic drug may delay a relapse, yet, when this happens, a more resistant trait emerges. Moreover, we estimate the expansion rate of the tumor boundary as well as the time of relapse, in terms of the resistance trait, the level of the nutrient, and the drug concentration. Finally, we propose an efficient drug schedule aiming at minimizing the growth rate of the most resistant trait. By combining the cytotoxic and cytostatic drugs, we demonstrate that the resistant cells can be eliminated.

Data-driven multiscale modeling of cell fate dynamics
Qing Nie, University of California, Irvine

Abstract: Cells make fate decisions in response to dynamic environmental and pathological stimuli as well as cell-to-cell communications. Recent technological breakthroughs have enabled to gather data in previously unthinkable quantities at single cell level, starting to suggest that cell fate decision is much more complex, dynamic, and stochastic than previously recognized. Multiscale interactions, sometimes through cell-cell communications, play a critical role in cell decision-making. Dissecting cellular dynamics emerging from molecular and genomic scale in single-cell demands novel computational tools and multiscale models. In this talk, I will present our recent works on analyzing single-cell molecular data, and their connections with cellular and spatial tissue dynamics. Our mathematical approaches bring together optimization, statistical physics, ODEs/PDEs, and stochastic simulations along with machine learning techniques. By utilizing our newly developed computational tools along with their close integrations with new datasets collected from our

experimental collaborators, we are able to investigate several complex systems during development and regeneration to uncover new mechanisms in cell fate determination.

Towards Open World Video Event Understanding - Flexible Representations, Commonsense Priors, and Self-Supervised Learning
Sudeep Sarkar, University of South Florida

Abstract: Events are central to the content of human experience. From the constant stream of the sensory onslaught, the brain segments, extracts, represents aspects related to events, and stores in memory for future comparison, retrieval, and re-storage. Contents of events consist of objects/people (who), location (where), time (when), actions (what), activities (how), and intent (why). Many deep learning-based approaches extract this information from videos. However, most methods cannot adapt much beyond what they were trained and are incapable of recognizing new events beyond what they were explicitly programmed or trained. The main limitation of current event analysis approaches is the implicit closed world assumption. The ability to support open world inference is limited by three main aspects: the underlying representation, the source of semantics, and the ability to continuously learn or adapt.
In this talk, I will focus on flexible representations, amenable for open-world, and self-supervised learning that is not dependent on the existence of a large amount of training data. We will see how Grenander's pattern theory-based canonical representation offers an elegant, flexible, compositional mechanism. It naturally models semantic connections between what is observed directly in the image and prior knowledge in large-scale commonsense knowledge bases, such as ConceptNet. The use of knowledge bases such as ConceptNet allows expanding the set of primary objects and actions to a very large (not infinite) set without the need for massive annotated training sets. And finally, if we have time, how predictive learning can be used to continuously learn how to segment a video into elementary event segments, again without training annotations.

Distinguished Panelist Talk

Recent developments in mixed finite element methods for stochastic Stokes and Navier-Stokes equations
Xiaobing Feng, University of Tennessee

Abstract: Besides the mathematical interests, stochastic Stokes and Navier-Stokes equations have been proposed to study turbulence flow under random forcing. Even in the simplest setting,their PDE solutions have very low regularity in time (and in space), which then poses a significant challenge for developing efficient and convergent numerical methods for the stochastic Stokes and Navier-Stokes equations. In particular, the most natural and popular class of numerical methods for those equations, namely mixed finite element methods, had not been proven to work. In this talk I shall present some recent developments in mixed finite element methods for the Stokes and Navier-Stokes equations with multiplicative noise. I shall highlight the establishment of the continuous and discrete stochastic inf-sup conditions and the strong convergence not only for the velocity approximation but also for the pressure approximation, as well as the new analysis techniques used to obtain these results. Numerical experiments will also be presented to validate the theoretical results.

Statistical Morphometrics in Life Sciences
Anuj Srivastava, University of South Florida

Abstract: Ever since D'Arcy Thompson's monumental work "On Growth and Form",
scientists have sought techniques to quantify shapes of biological objects and to help understand their roles in larger biological systems. This quest has been accelerated by a revolution in techniques that probe the chemical, structural, and dynamical nature of molecules, cells, tissues, and organs across scales. Such structured data defies past techniques from Euclidean statistics, and requires careful constructions of representations, models, and analyses. I will provide some examples of modeling and analyzing biological structures using a combination of geometry, statistics, and computational solutions.

Trends and opportunities in life sciences
Guo-Wei Wei, Michigan State University

Abstract: Life science or biological science is believed to be the last forefront of natural sciences. It became molecular in the 1960s and assumed an omics dimension around the dawn of the millennium. The exponential growth of biological data has paved the way for biological sciences to undertake another historical transition from qualitative, phenomenological and descriptive to quantitative, analytical and predictive. This transition gives rise to unprecedented opportunities for mathematicians. Mathematics is indispensable for understanding the rules of life. For example, differential geometry, algebraic geometry, algebraic topology, knot theory, combinatorics, topological graph, and spectral graph are powerful tools for the abstraction and simplification of complex biomolecules, such as proteins, DNA, and RNA, and for revealing their structure-function relationship. Dynamical systems and multiscale analysis are essential techniques for analyzing and elucidating molecular, organelle, and cellular motion and dynamics. Partial differential equations are vital for understanding the transport of ions, molecules, organelles, and cells in the biological environment. Additionally, mathematics is all-known for its strong presence in evolution, population, neuroscience, ecology, virology, immunology, and physiology, which are becoming molecular and data-driven nowadays. Scientific computing facilitates various mathematical approaches to biological sciences. Mathematics underpins machine learning that is the fourth paradigm of biological sciences. Currently, mathematicians are working more closely with experimentalists than ever before.

Invited Talks

Sub-epidemic modeling framework for short-term forecasting epidemic waves
Gerardo Chowell, Georgia State University

Abstract: Simple phenomenological growth models can be useful for estimating transmission parameters and forecasting epidemic trajectories. However, most existing phenomenological growth models only support single-peak outbreak dynamics whereas real epidemics often display more complex transmission trajectories. Methods: We develop and apply a novel sub-epidemic modeling framework that supports a diversity of epidemic trajectories including stable incidence patterns with sustained or damped oscillations to better understand and forecast epidemic outbreaks. We describe how to forecast an epidemic based on the premise that the observed coarse-scale incidence can be decomposed into overlapping sub-epidemics at finer scales. We evaluate our modeling framework using three outbreak datasets: Severe Acute Respiratory Syndrome (SARS) in Singapore, plague in Madagascar, and the ongoing Ebola outbreak in the Democratic Republic of Congo (DRC) and four performance metrics.
Results: The sub-epidemic wave model outperforms simpler growth models in short-term forecasts based on performance metrics that account for the uncertainty of the predictions namely the mean interval score (MIS) and the coverage of the 95% prediction interval. For example, we demonstrate how the sub-epidemic wave model successfully captures the 2-peak pattern of the SARS outbreak in Singapore. Moreover, in short-term sequential forecasts the sub-epidemic model was able to forecast the second surge in case incidence for this outbreak, which was not possible using the simple growth models. Furthermore, our findings support the view that the national incidence curve of the Ebola epidemic in DRC follows a stable incidence pattern with periodic behavior that can be decomposed into overlapping sub-epidemics.
Conclusions: Our findings highlight how overlapping sub-epidemics can capture complex epidemic dynamics, including oscillatory behavior in the trajectory of the epidemic wave. This observation has significant implications for interpreting apparent noise in incidence data where the oscillations could be dismissed as a result of overdispersion, rather than an intrinsic part of the epidemic dynamics. Unless the oscillations are appropriately modeled, they could also give a false positive, or negative, impression of the impact from public health interventions. These preliminary results using sub-epidemic models can help guide future efforts to better understand the heterogenous spatial and social factors shaping sub-epidemic patterns for other infectious diseases.

Machine Learning in Biomedical Research – Early Detection of Disease via Telemetry Signals
Juan B. Gutiérrez, University of Texas at San Antonio

Abstract: Machine learning can solve problems that traditional methods in mathematics are simply unable to tackle. The context for this talk is malaria, an infectious disease caused by members of the Plasmodium genus. There is a lapse of between one and two weeks after infection, called the liver stage, in which detection of malaria is not possible with current technology. Once malaria symptoms begin, the disease might turn deadly within 24 hours, hence the urgency to develop early detection methods. In this talk, I will present high-frequency physiological data captured from telemetry devices surgically implanted in Macaca mulatta and M. fascicularis prior to and during infection with Plasmodium knowlesi sporozoites. The challenges of analyzing this type of data are enormous, and include but are not limited to: selection of method of analysis, data capture, data storage and transmittal, reproducibility of results, etc. Particularly, we will talk about deep learning can be used for this problem. Our results show for the first time that host physiological perturbations can be detected while malaria parasites are multiplying in the liver, a step that precedes blood-stage infections and clinical symptomology. These findings demonstrate that machine learning can be deployed successfully to address problems for which we lack mathematical tools, and although we obtain knowledge without understanding, it is precisely our inability to comprehend the characteristics of the phenomenon detected by machines what opens pathways for the advance of mathematics.

Harnessing the power of genomics data sciences with Machine Learning
Rays H.Y. Jiang, University of South Florida

Abstract: Biological science is in 'big data' era. Particularly, genomics data, such as 23&Me, have entered commercial sectors with projected exponential growth. This bio data revolution is enabled by the novel technology development of miniaturization, standardization and massive production. To face the challenge of outpouring data production, Artificial Intelligence (AI) approaches such as Machine learning (ML), knowledge representation, and Nature Language Processing (NLP) are poised to solve the genomics problems of large volume and high dimension data. At USF (University of South Florida) genomics, we have the unique capacity of integrating cutting-edge genomics, engineering, and domain knowledge to produce high volume of novel genomics data, in the field of infectious diseases, developmental biology and evolutionary biology. We currently are actively solving data problems of 1) very high dimensions of single-cell biology with Manifold Learning 2) unique evolutionary microbiota data with ML 3) large scale network analysis gene function data such as CRISPR and gene expressions. I will review the current status, challenges and future directions of translating genomics big data into actionable knowledge to propel biological and health sciences.

Elastic Hyper-alignment of fMRI Signals
Shantanu Joshi, University of California, Los Angeles

Abstract: This talk presents approaches for temporal matching of fMRI signals. It presents applications for functional magnetic resonance imaging (fMRI) time course and spectral alignment. We show elastic alignment of both amplitude and phase of the fMRI time courses as well as their power spectral densities. Experimental results show significant increases in pairwise node to node correlations and coherences following alignment. Additionally, we show results for task based fMRI signals, where we see improved power of detection of clusters and activations for single subject data.

Thermal Effects in General Diffusion with Biological Applications
Chun Liu, Illinois Institute of Technology

Abstract: All biological activities involve transport and distribution of ions and charged particles in specific biological environments. Moreover, the thermal effects are the key for these activities. In this talk, I will

introduce several extended general diffusion systems motivated by the study of ion channels and ionic solutions in biological cells. A general framework is established, which incorporates the energetic variational approaches (EnVarA) with various thermodynamics and kinematic conditions. In particular, we will focus on the interactions between different species, the boundary effects and the temperature effects.

Machine Learning and Transport Simulations for Groundwater Anomaly Detection
James Liu, Colorado State University

Abstract: In this talk, we present studies on models and algorithms for groundwater anomaly detection. Specifically, conductivity along with four other surrogates are used for identifying anomaly in groundwater, the one-class support vector machine (SVM) technique is utilized for model training, and real data from "Colorado Water Watch" is used for testing the models and algorithms. Design of code modules in Python is briefly discussed. Since groundwater contamination rarely happens in reality, we also use synthetic data from numerical simulations of flow and transport in porous media to test the anomaly detection code modules. This is based on the joint work with Ken Carlson, Jianli Gu, and Huishu Li at Colorado State University.

A Bayesian Gamma-Negative-Binomial Model for Single-Cell RNA-Seq Data
Xiaoning Qian, Texas A&M University

Abstract: A generative hierarchical gamma-negative-binomial (hGNB) model is developed to analyze single-cell RNA-sequencing (scRNA-seq) data, obviating the need for explicitly modeling zero inflation in many existing methods. Due to its generative nature, hGNB can account for covariate effects at both the gene and cell levels to identify complex latent representations of scRNA-seq data, without the need for commonly adopted pre-processing steps such as normalization. Efficient Bayesian model inference is derived by exploiting conditional conjugacy via novel data augmentation techniques. Experimental results on both simulated data and several real-world scRNA-seq datasets will be presented to show the potential of hGNB.

A parametric bootstrap region construction for the mean elastic shape
Justin D Strait, University of Georgia

Abstract: Visualization is an integral component of statistical shape analysis, where the goal is to perform inference on shapes of objects. When interested in identifying shape variation, one typically performs principal component analysis (PCA) to decompose total variation into orthogonal directions of variation. In many cases, shapes observe multiple sources of variation; using PCA to visualize requires decomposition into several plots displaying each mode of variation, without the ability to understand how these components work together. I propose a parametric construction (according to a model-based bootstrap) for a high density region for the elastic shape mean, with the goal of also producing a succinct visual summary of this region. The use of elastic shape representations allows for optimal matching of shape features, yielding more appropriate estimation of shape variation than some other approaches. Discussion of visualization issues is included. The proposed region is estimated for simulated data, as well common shapes from the well-known MPEG-7 dataset.

Geometric methods in human movement analysis
Pavan Turaga, Arizona State University

Abstract: In this talk, we will discuss problems involving human movement analysis, where we motivate the need for mathematical approaches rooted in differential geometry and topology. We discuss recent work in non-linear dynamical analysis as applied to human activity modeling where we propose to characterize dynamical attractors via their geometric and topological properties. We demonstrate results on activity recognition and scene analysis problems where these methods provide a well-grounded general purpose

framework. These methods are shown to work well in a variety of different dynamical time-series databases with minimal changes to the underlying framework. We also present preliminary interdisciplinary work and emerging opportunities at the intersection of geometric computing and real-time interactive feedback systems for mobility and balance-related disorders.

Can AI discover the drugs of the future?
Guowei Wei, Michigan State University

Abstract: The dominant win of Google's Alphafold in the latest Critical Assessment of Structure Prediction (CASP) competition has ushered a new era of scientific discovery. Researchers are excited about what the future may hold for drug discovery. Artificial intelligence (AI) might make new drug discovery significantly faster and cheaper. This could be particularly beneficial to patients with rare medical ailments, for whom drug discovery is currently not profitable, or for those whose medical ailments currently cannot be effectively treated with drugs, such as Alzheimer's disease. However, drug design is much more complex than protein folding prediction. Due to the structural complexity of protein-drug interactions, the high dimensionality of drug candidates' chemical space, and the involved molecular simulation and deep learning (DL), even all the world's computers put together do not have enough power to design drug automatically. In my lab, we tackle these challenges mathematically. Our work focuses on reducing the geometric complexity and degrees of freedom of protein-drug complexes for AI and DL, such as generative adversarial neural networks (GANs). We have introduced differential geometry, algebraic topology, and graph theory to obtain high-level abstractions of protein-drug complexes and thus enable GANs to handle excessively large datasets in drug discovery. Our mathematical AI has made us a top competitor in D3R Grand Challenges, a worldwide competition series in computer-aided drug design and discovery in the past three years.

Risk assessments on eradication of aquatic invasive species
Yanyu Xiao, University of Cincinnati

Abstract: In the work, we evaluate the performance of machine learning approaches for predicting successful eradication of aquatic invasive species and assess the extent to which eradication of an invasive species depends on the various specific ecological features of the target ecosystem and/or features that characterize the planned intervention.

Finite element methods with discontinuous approximations
Xiu Ye, University of Arkansas at Little Rock

Abstract: In this presentation, different finite element methods with discontinuous approximations will be discussed including IPDG, HDG and specially WG finite element methods as well as the relations between them. In addition, new stabilizer free discontinuous finite element methods will be introduced.